

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
 Data File : BP019746.D
 Acq On : 16 Feb 2024 15:50
 Operator : MA/JU
 Sample : P1440-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TW-3

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019746.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	324	329	337	rVB	86017	128463	1.47%	0.175%
2	5.399	387	393	399	rBV	133379	205946	2.35%	0.281%
3	5.475	399	406	417	rVB	1000616	1468111	16.75%	2.005%
4	6.534	556	586	594	rBV2	151296	641257	7.32%	0.876%
5	7.075	671	678	692	rVB	614961	1033931	11.80%	1.412%
6	7.899	812	818	825	rBV	262020	429148	4.90%	0.586%
7	8.640	936	944	957	rBV	661442	1051220	11.99%	1.436%
8	9.075	1007	1018	1030	rBV	854564	1505783	17.18%	2.057%
9	9.228	1033	1044	1057	rVB	195755	343214	3.92%	0.469%
10	9.769	1131	1136	1154	rBV	29470	122481	1.40%	0.167%
11	10.057	1176	1185	1194	rBV3	62897	136071	1.55%	0.186%
12	10.699	1288	1294	1306	rVB	302328	523760	5.98%	0.715%
13	11.028	1344	1350	1356	rBV	67964	131839	1.50%	0.180%
14	11.740	1462	1471	1490	rBV	947983	1586766	18.10%	2.167%
15	12.263	1552	1560	1577	rBV	624160	954105	10.89%	1.303%
16	12.857	1654	1661	1672	rBV5	89567	195672	2.23%	0.267%
17	12.993	1679	1684	1696	rVB3	55148	123482	1.41%	0.169%
18	13.163	1705	1713	1718	rBV	2208332	3332417	38.02%	4.551%
19	13.210	1718	1721	1728	rVV	354254	559161	6.38%	0.764%
20	13.275	1728	1732	1740	rVB3	63186	108512	1.24%	0.148%
21	13.675	1793	1800	1814	rBV	1291637	1886723	21.53%	2.577%
22	14.187	1881	1887	1902	rBV	578582	827905	9.45%	1.131%
23	14.534	1941	1946	1952	rBV	416087	624268	7.12%	0.853%
24	14.593	1952	1956	1970	rVB	933724	1309126	14.94%	1.788%
25	14.993	2015	2024	2034	rBV	702009	1101383	12.57%	1.504%
26	15.298	2066	2076	2088	rBV	1025217	1448463	16.53%	1.978%
27	15.710	2140	2146	2157	rVB	1044608	1401144	15.99%	1.914%
28	15.969	2184	2190	2196	rBV	488838	669817	7.64%	0.915%
29	16.040	2196	2202	2207	rVV	1697147	2625056	29.95%	3.585%
30	16.087	2207	2210	2220	rVB	244225	354405	4.04%	0.484%
31	16.434	2263	2269	2276	rBV	436837	576840	6.58%	0.788%
32	16.716	2311	2317	2325	rBV	300555	423991	4.84%	0.579%
33	17.010	2362	2367	2374	rBV	1271687	1750572	19.97%	2.391%
34	17.245	2402	2407	2410	rBV	69841	101389	1.16%	0.138%
35	17.292	2410	2415	2426	rVB	496834	754021	8.60%	1.030%
36	17.392	2426	2432	2438	rBV	6661595	8764736	100.00%	11.971%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
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37	17.563	2456	2461	2473	rBV	1116710	1567190	17.88%	2.140%
38	17.687	2478	2482	2488	rBV	85395	119658	1.37%	0.163%
39	17.992	2527	2534	2543	rBV	169124	239404	2.73%	0.327%
40	18.104	2548	2553	2561	rBV	575555	727109	8.30%	0.993%
41	18.192	2563	2568	2578	rVV2	269970	384779	4.39%	0.526%
42	18.469	2610	2615	2622	rBV	663476	823013	9.39%	1.124%
43	18.804	2666	2672	2677	rBV	1560890	1976476	22.55%	2.699%
44	18.916	2686	2691	2701	rBV	1624949	2111692	24.09%	2.884%
45	19.281	2749	2753	2756	rBV3	68914	108519	1.24%	0.148%
46	19.345	2759	2764	2771	rVV	1288594	1639231	18.70%	2.239%
47	19.428	2774	2778	2787	rVV2	129519	193921	2.21%	0.265%
48	19.569	2798	2802	2808	rBV2	84472	131093	1.50%	0.179%
49	19.675	2816	2820	2823	rBV	238096	282051	3.22%	0.385%
50	19.722	2823	2828	2831	rVV	1343232	1616760	18.45%	2.208%
51	19.763	2831	2835	2842	rVB	519365	650720	7.42%	0.889%
52	19.863	2846	2852	2862	rBV2	4716972	6208012	70.83%	8.479%
53	19.969	2866	2870	2879	rBV	671184	882277	10.07%	1.205%
54	20.063	2884	2886	2896	rVB	888112	1194361	13.63%	1.631%
55	20.404	2939	2944	2952	rBV	1565204	1808609	20.64%	2.470%
56	20.645	2982	2985	2990	rVB	118062	144834	1.65%	0.198%
57	20.757	2999	3004	3006	rBV	1138172	1323491	15.10%	1.808%
58	20.875	3017	3024	3036	rBV2	607655	1013396	11.56%	1.384%
59	20.975	3037	3041	3046	rBV	283294	370659	4.23%	0.506%
60	21.028	3047	3050	3055	rVB	219718	250359	2.86%	0.342%
61	21.110	3059	3064	3075	rVB2	730418	1150547	13.13%	1.571%
62	21.339	3099	3103	3107	rBV	506192	581254	6.63%	0.794%
63	21.386	3107	3111	3118	rVB	779032	1062674	12.12%	1.451%
64	21.569	3139	3142	3151	rVB	218200	269971	3.08%	0.369%
65	21.663	3154	3158	3165	rVB	991074	1256394	14.33%	1.716%
66	22.010	3213	3217	3227	rVB	597680	795197	9.07%	1.086%
67	22.310	3264	3268	3276	rBV2	124319	252220	2.88%	0.344%
68	22.392	3278	3282	3290	rVB	180654	270334	3.08%	0.369%
69	22.680	3326	3331	3335	rBV	236522	392634	4.48%	0.536%
70	23.086	3395	3400	3408	rVB	436091	719697	8.21%	0.983%
71	23.545	3474	3478	3488	rVB	241269	447549	5.11%	0.611%
72	23.810	3517	3523	3530	rVB	523644	1050138	11.98%	1.434%

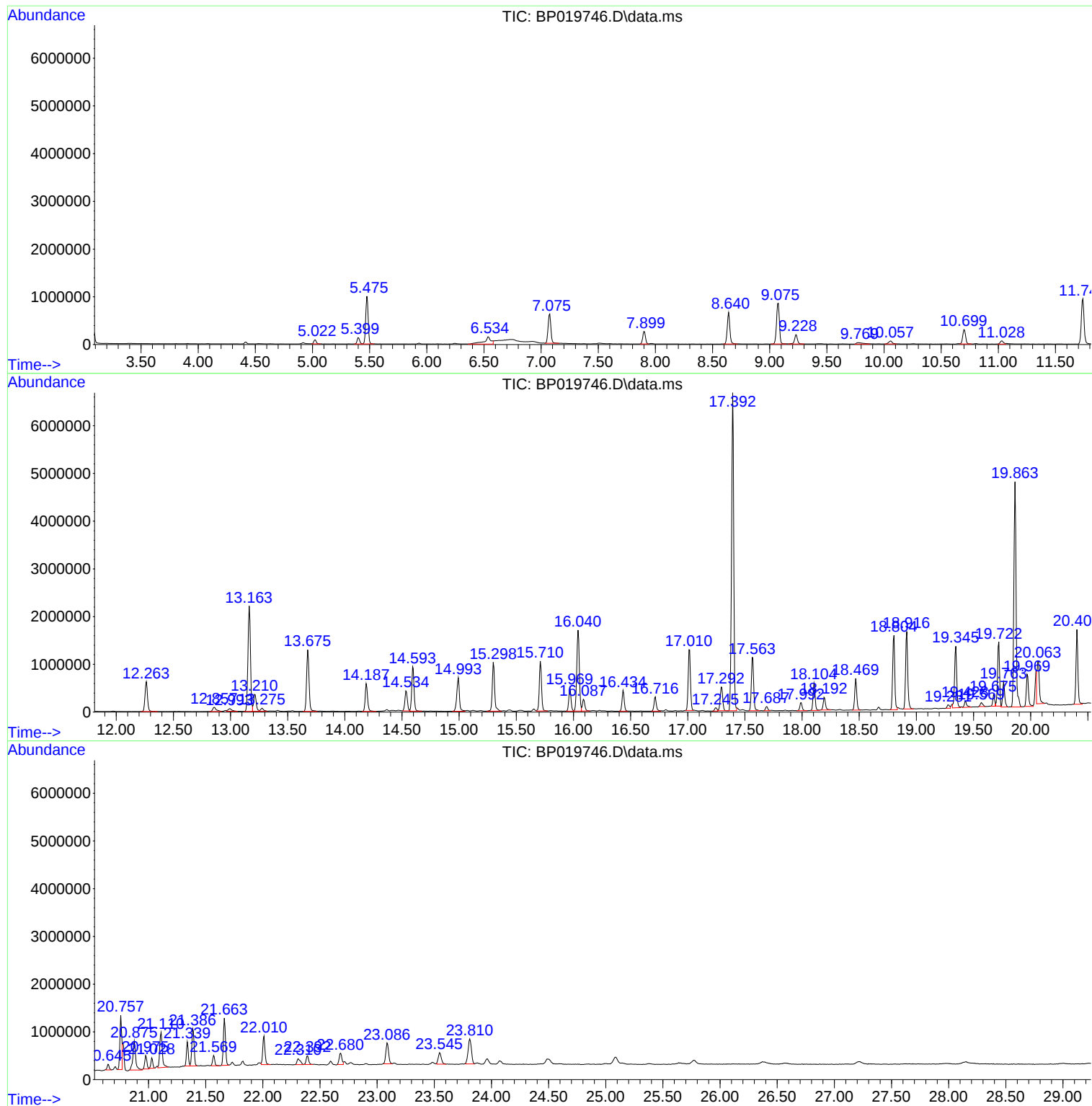
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Operator : MA/JU
Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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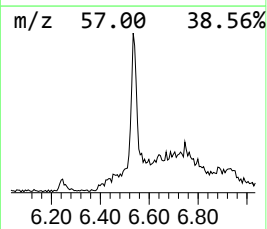
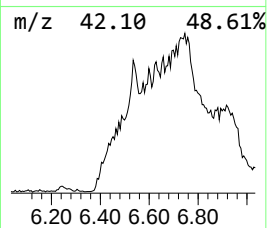
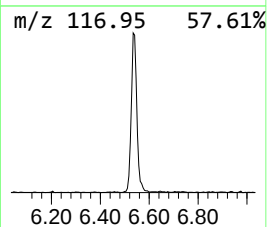
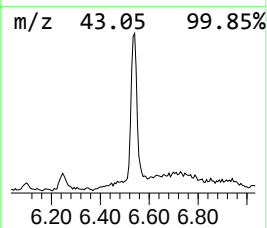
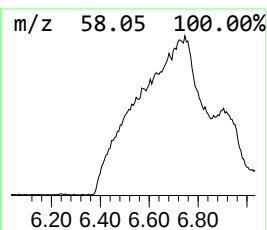
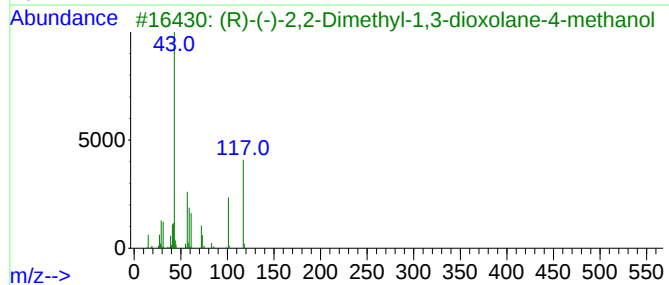
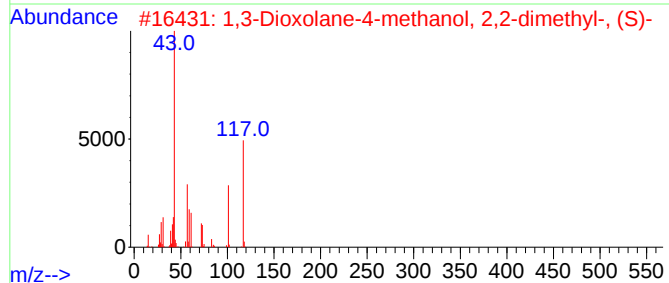
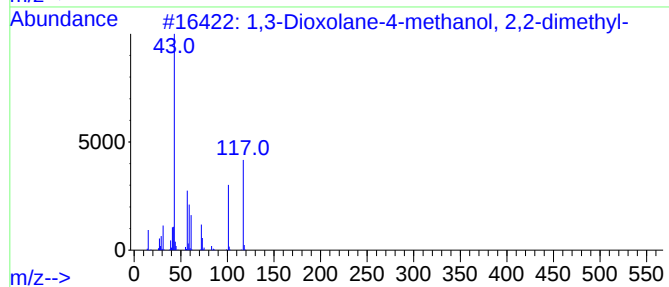
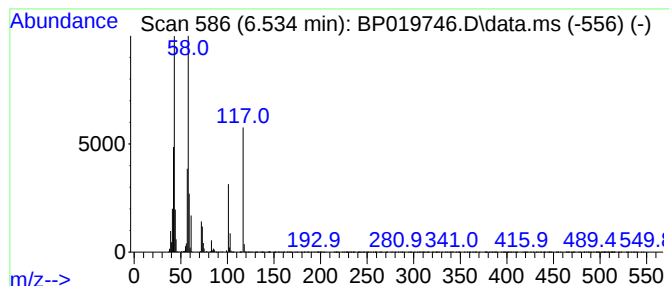
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.534 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.534	29.89 ng	641257	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	000100-79-8	38
2			1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	022323-82-6	38
3			(R)-(-)-2,2-Dimethyl-1,3-dioxola...	132	C6H12O3	014347-78-5	38
4			Betaine	117	C5H11NO2	000107-43-7	33
5			2(5H)-Furanone, 3-chloro-5-((dim...	203	C9H14ClNO2	104502-43-4	28



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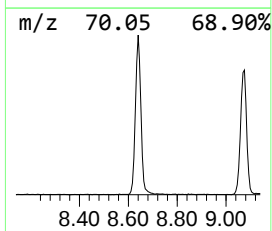
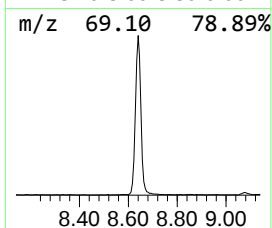
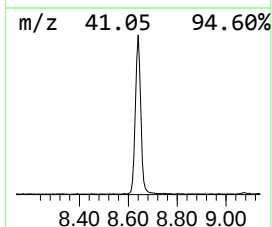
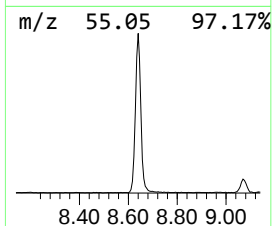
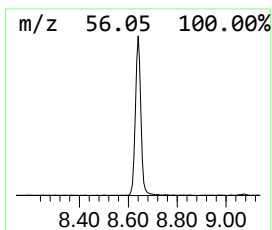
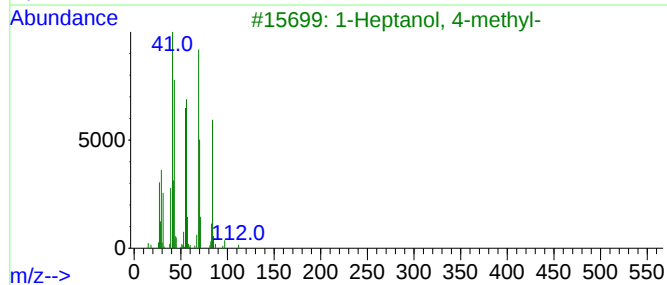
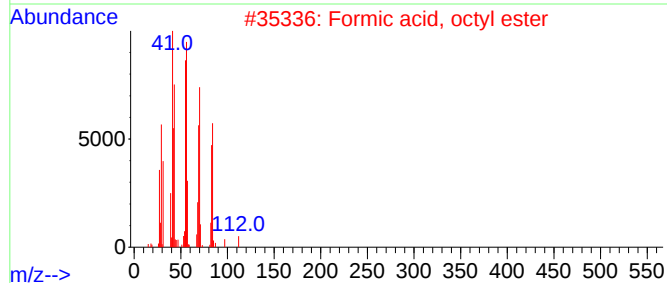
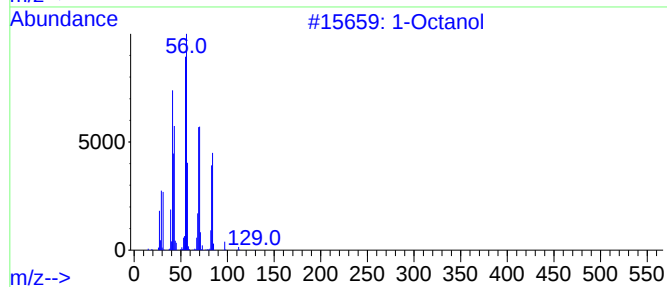
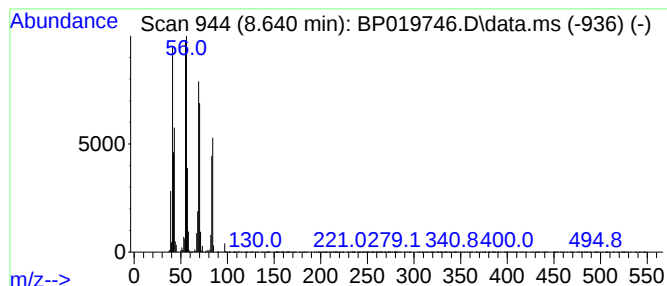
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Octanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.640	48.99 ng	1051220	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	64
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	59
3			1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	47
4			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	43
5			Formic acid, heptyl ester	144	C8H16O2	000112-23-2	43



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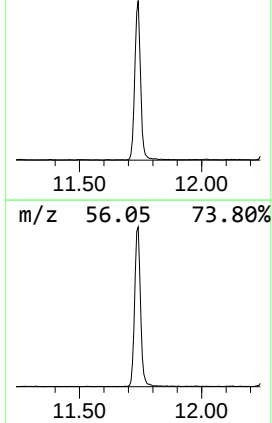
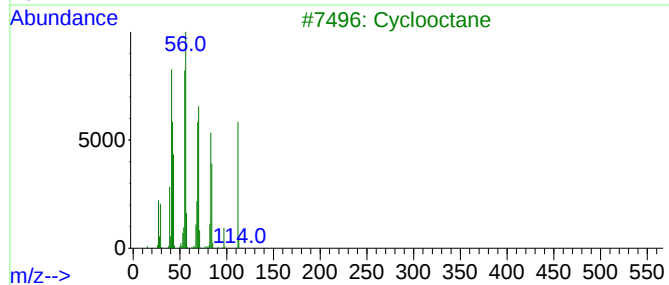
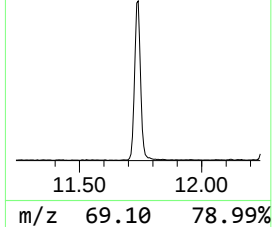
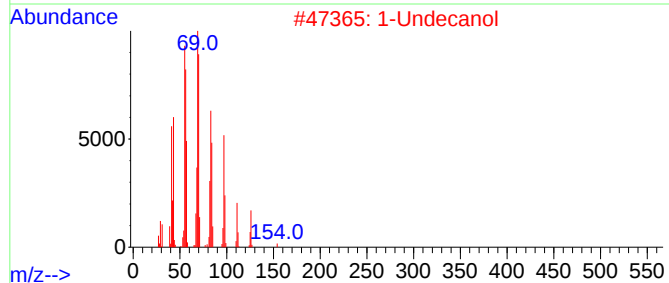
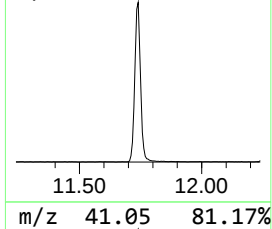
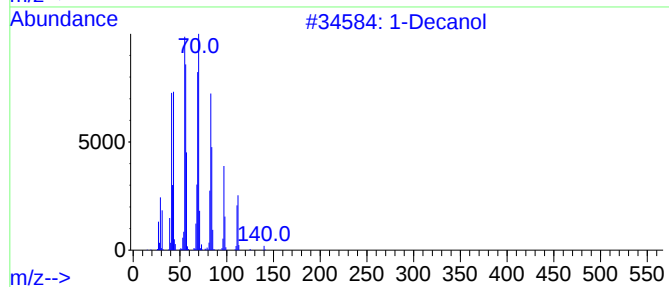
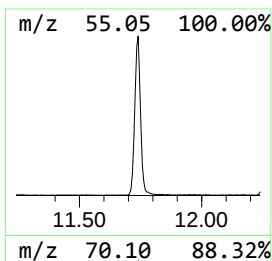
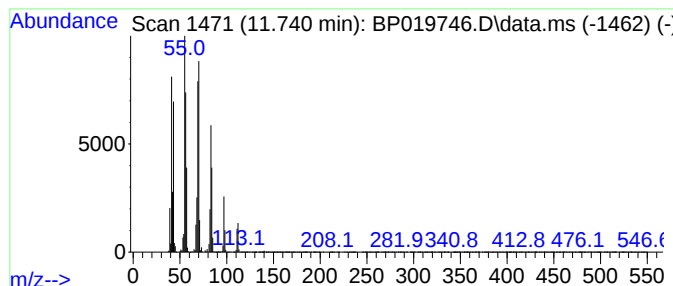
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.740	60.59 ng	1586770	Naphthalene-d8	10.699	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol	158	C10H22O	000112-30-1	91
2	1-Undecanol	172	C11H24O	000112-42-5	86
3	Cyclooctane	112	C8H16	000292-64-8	62
4	1-Nonene	126	C9H18	000124-11-8	55
5	Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	52



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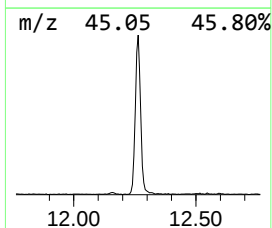
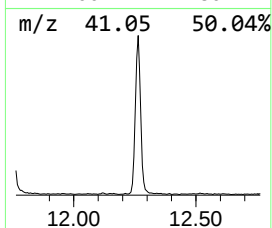
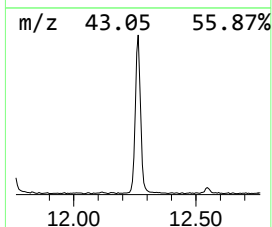
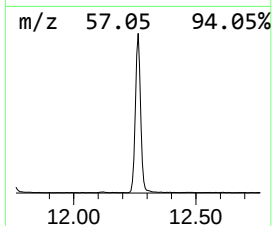
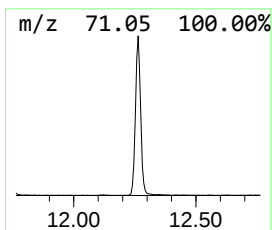
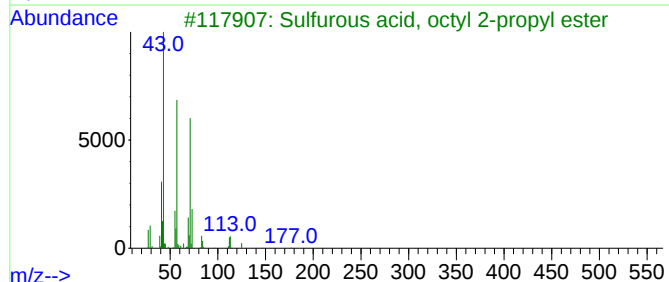
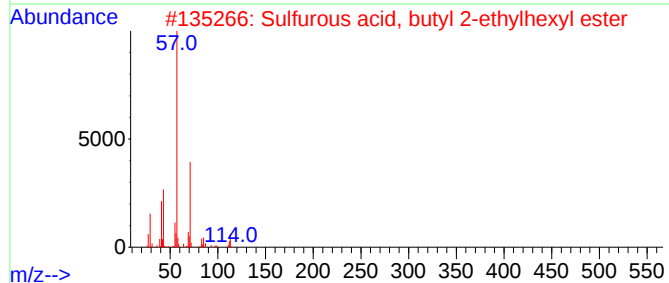
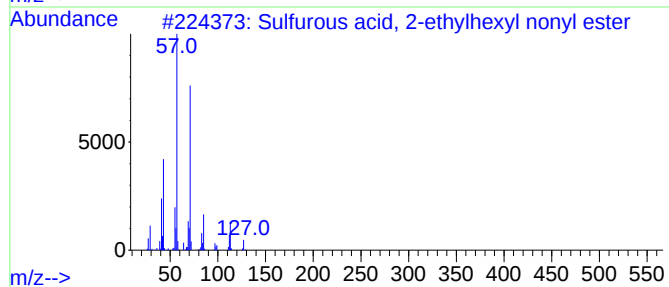
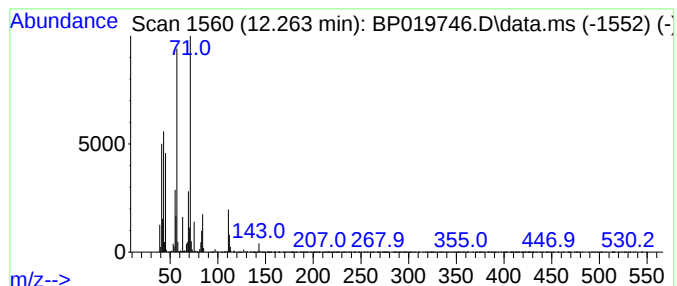
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.263 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.263	36.43 ng	954105	Naphthalene-d8	10.699	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	47
2	Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	47
3	Sulfurous acid, octyl 2-propyl e...	236	C11H24O3S	1000309-11-9	47
4	Methylamine, N-(1-methylhexylide...	127	C8H17N	022058-71-5	43
5	Octane, 3-ethyl-	142	C10H22	005881-17-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
Operator : MA/JU
Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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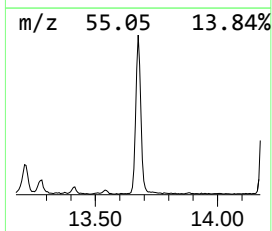
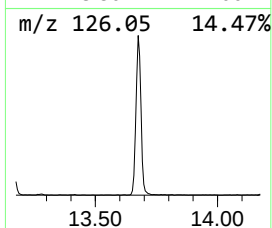
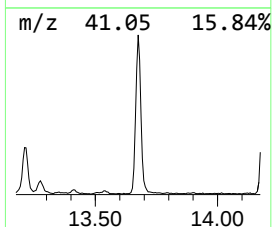
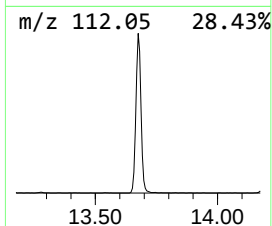
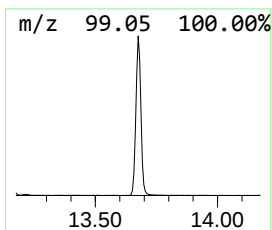
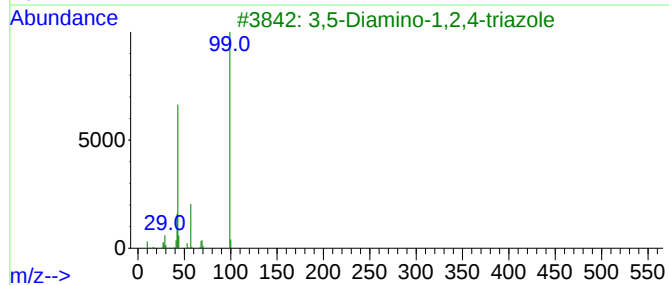
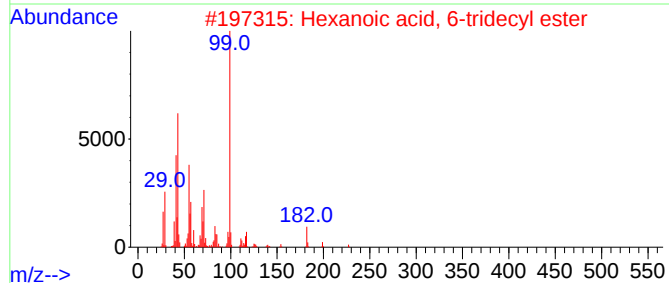
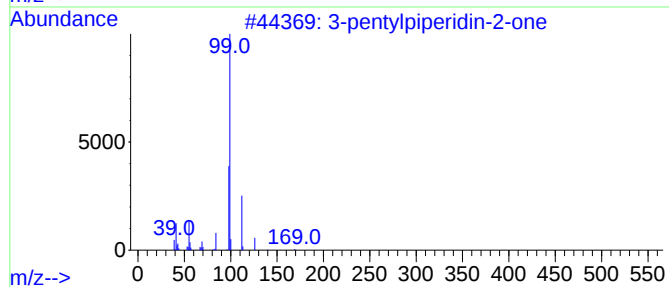
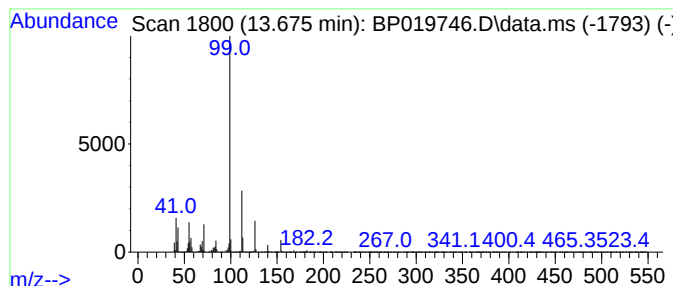
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-pentylpiperidin-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.675	60.45 ng	1886720	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-pentylpiperidin-2-one	169	C10H19NO	1000441-61-6	64
2			Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	53
3			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	43
4			Spiro[1,3-dioxolane-2,1'(4'H)-na...	210	C12H18O3	021727-93-5	40
5			2(3H)-Furanone, dihydro-5-methyl...	156	C9H16O2	010200-21-2	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
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Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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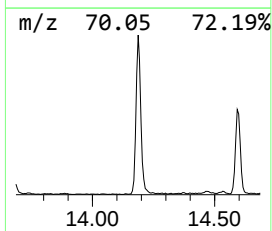
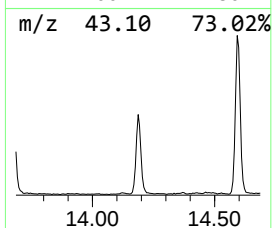
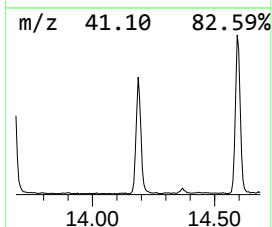
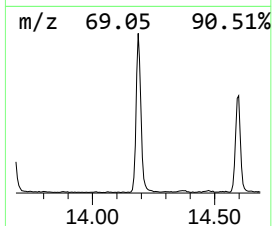
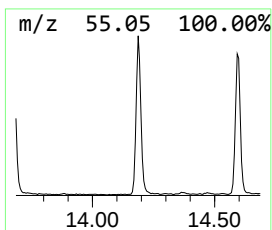
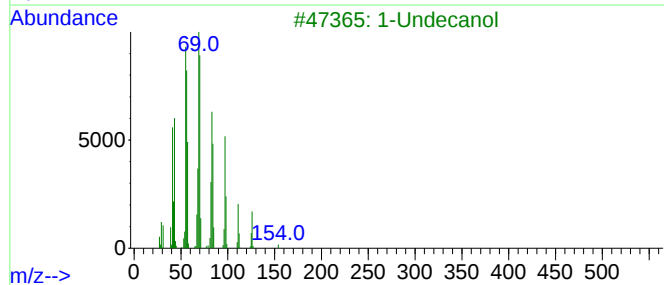
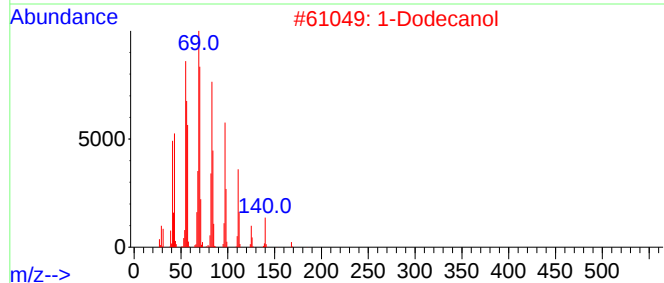
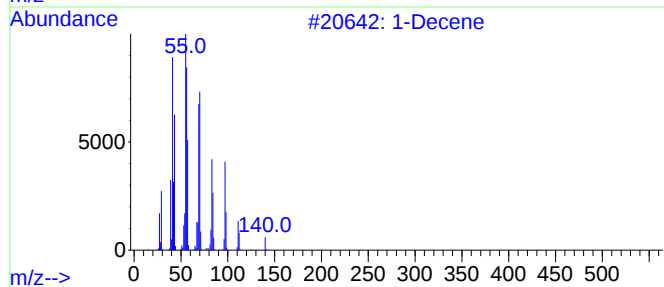
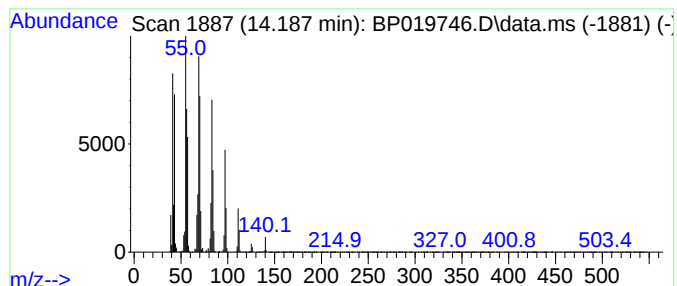
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Decene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.187	26.52 ng	827905	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decene	140	C10H20	000872-05-9	96
2			1-Dodecanol	186	C12H26O	000112-53-8	91
3			1-Undecanol	172	C11H24O	000112-42-5	91
4			Cetene	224	C16H32	000629-73-2	91
5			Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
Operator : MA/JU
Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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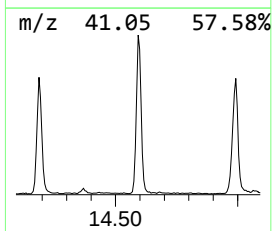
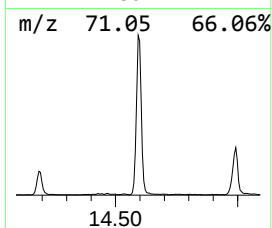
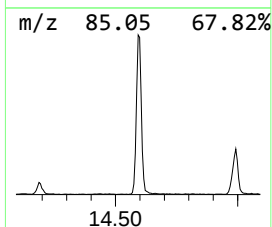
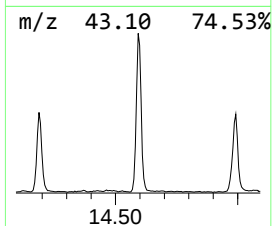
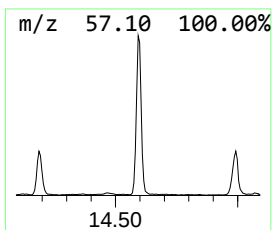
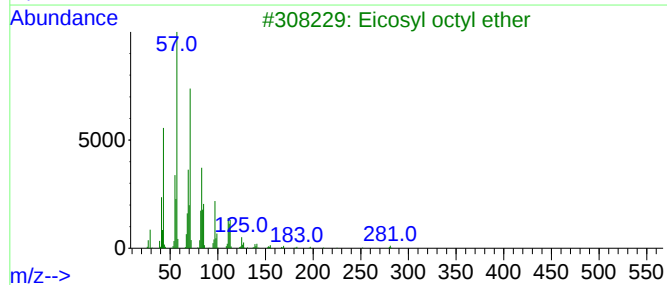
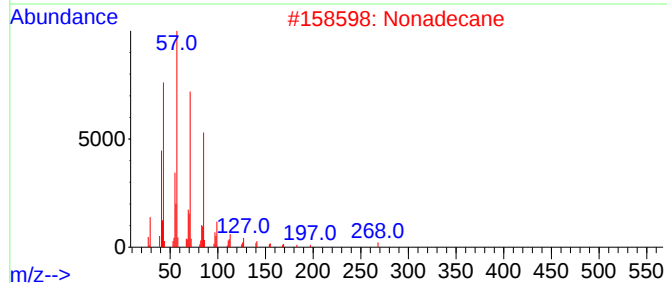
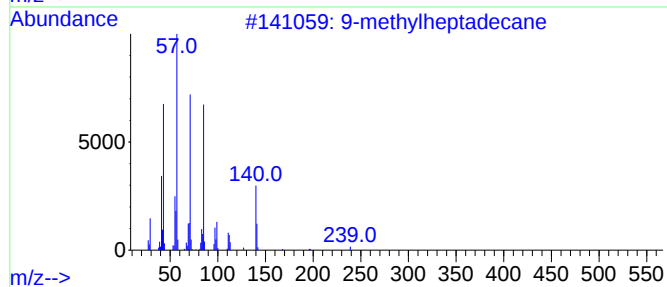
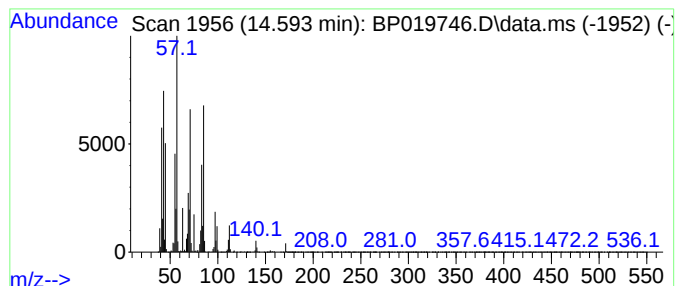
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown14.593 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.593	41.94 ng	1309130	Acenaphthene-d10	14.534

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-methylheptadecane	254	C18H38	026741-18-4	46	
2	Nonadecane	268	C19H40	000629-92-5	46	
3	Eicosyl octyl ether	410	C28H58O	1000406-38-8	46	
4	Hexadecyl octyl ether	354	C24H50O	1000406-38-6	46	
5	Decyl isobutyl ether	214	C14H30O	1010406-32-5	46	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
Operator : MA/JU
Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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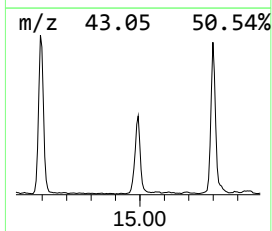
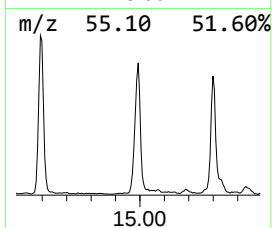
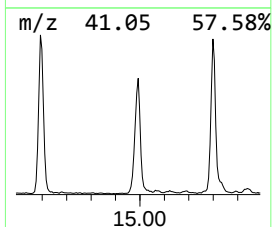
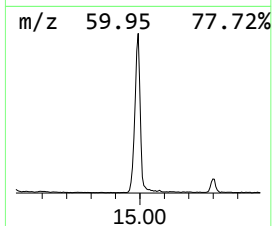
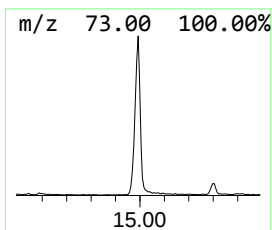
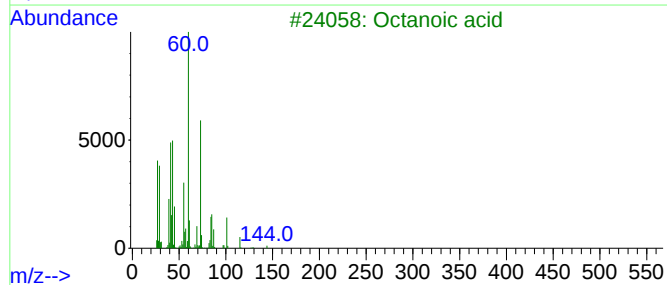
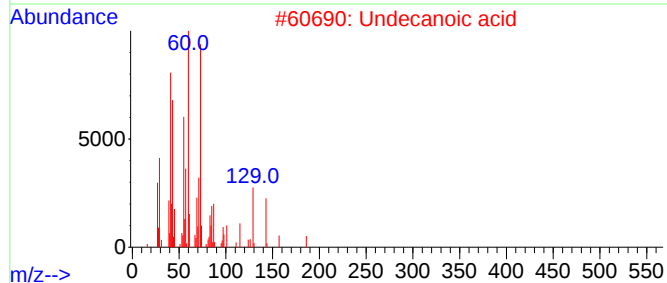
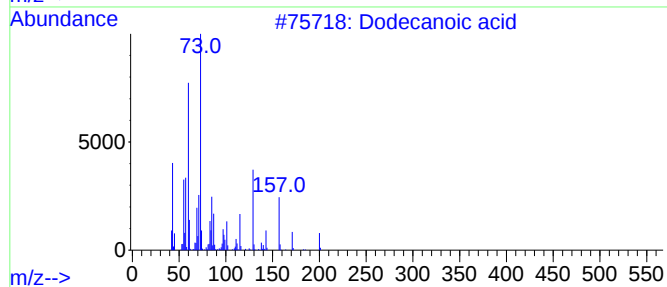
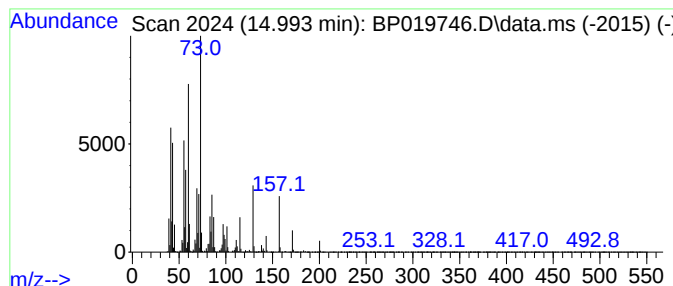
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Dodecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.993	35.29 ng	1101380	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	96
2			Undecanoic acid	186	C11H22O2	000112-37-8	59
3			Octanoic acid	144	C8H16O2	000124-07-2	49
4			Nonanoic acid	158	C9H18O2	000112-05-0	46
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
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Sample : P1440-05
Misc :
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Instrument :
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ClientSampleId :
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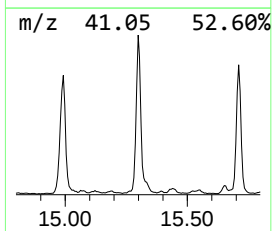
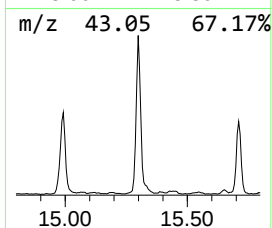
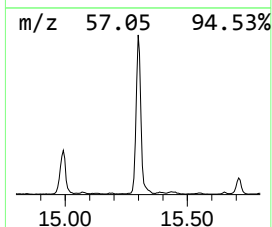
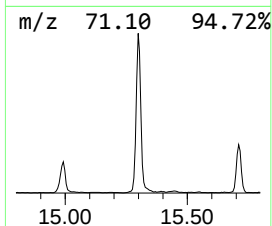
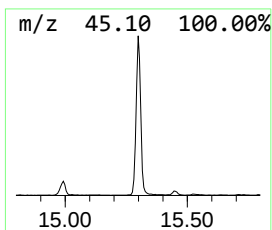
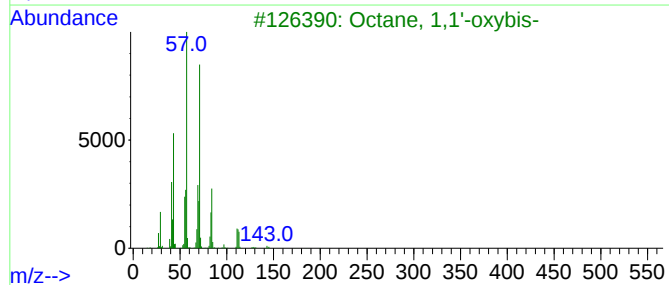
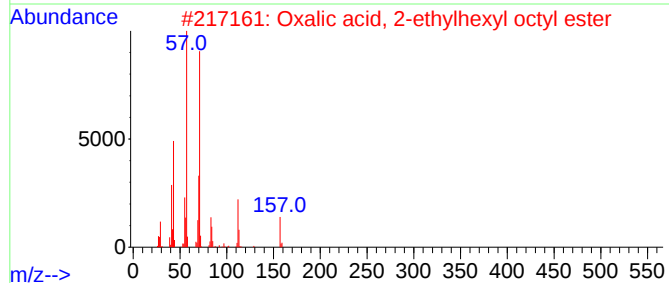
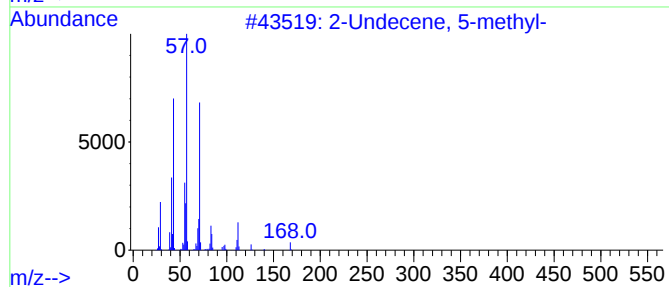
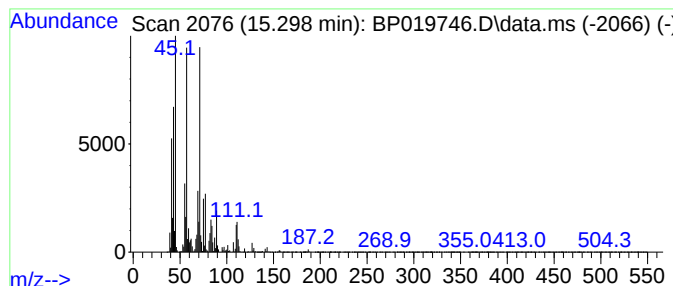
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown15.298 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	46.41 ng	1448460	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecene, 5-methyl-		168	C12H24	056851-34-4	27	
2	Oxalic acid, 2-ethylhexyl octyl ...		314	C18H34O4	1000309-39-1	27	
3	Octane, 1,1'-oxybis-		242	C16H34O	000629-82-3	27	
4	Sulfurous acid, butyl octyl ester		250	C12H26O3S	1000309-17-5	27	
5	2-Decanol		158	C10H22O	001120-06-5	22	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
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ClientSampleId :
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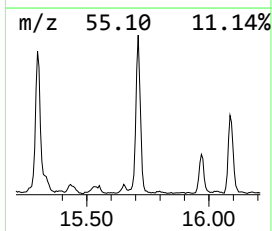
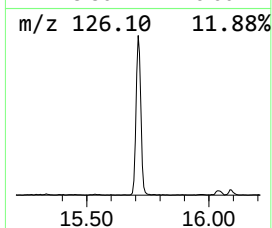
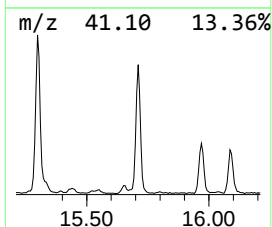
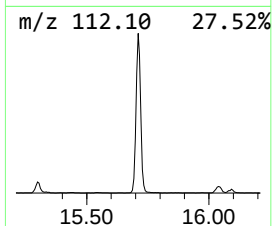
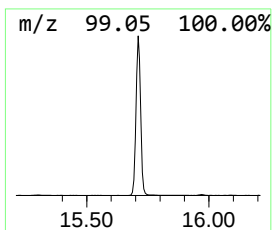
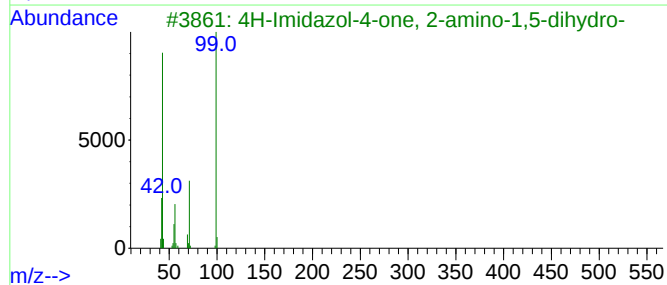
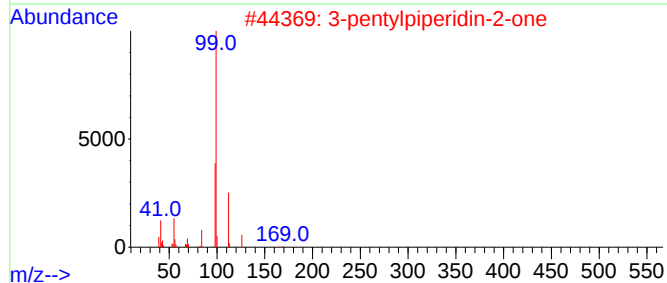
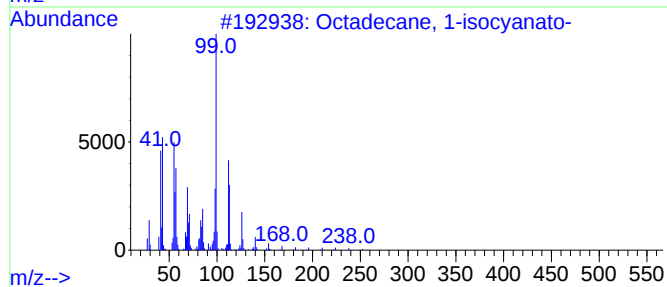
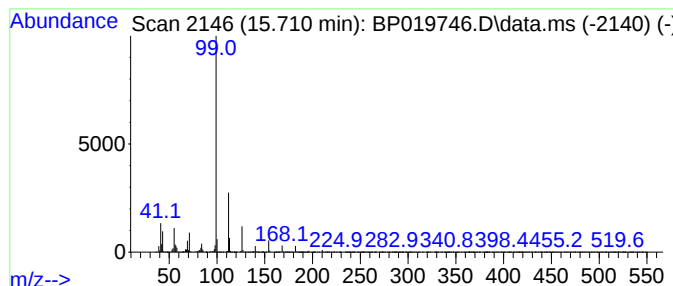
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octadecane, 1-isocyanato- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.710	44.89 ng	1401140	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-isocyanato-	295	C19H37NO	000112-96-9	72
2			3-pentylpiperidin-2-one	169	C10H19NO	1000441-61-6	64
3			4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	50
4			Hexanoic acid, 3-fluorophenyl ester	210	C12H15FO2	1000330-93-1	50
5			4-Methyl-2-(4-methyl-6-oxo-1-oxa...	214	C12H22O3	101153-83-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
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ClientSampleId :
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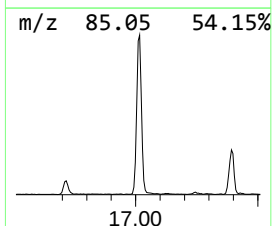
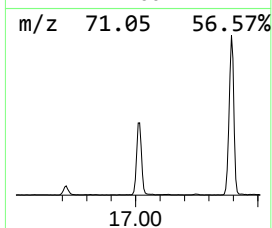
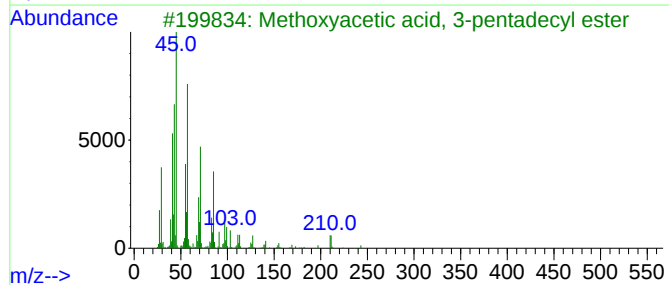
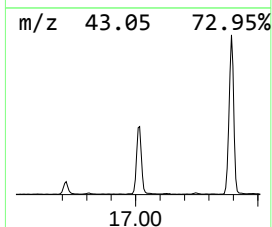
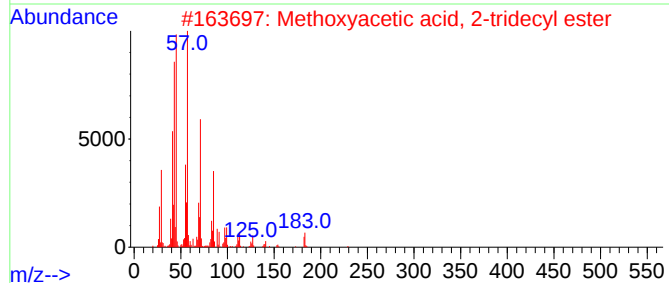
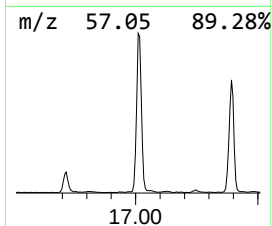
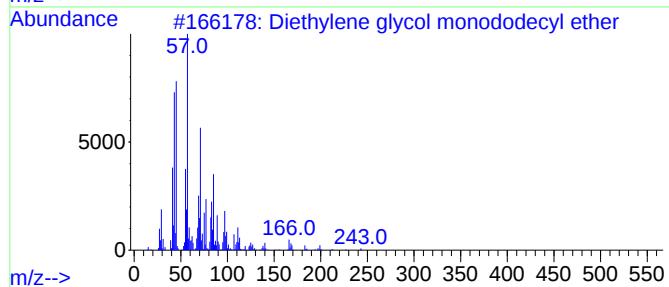
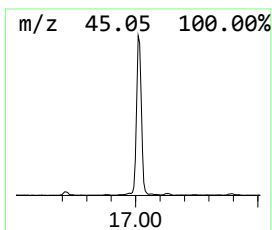
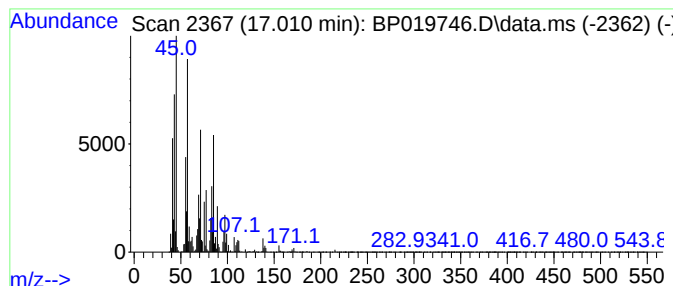
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Diethylene glycol monododec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.010	46.43 ng	1750570	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol monododecyl ether	274	C16H34O3	003055-93-4	72
2			Methoxyacetic acid, 2-tridecyl e...	272	C16H32O3	1000282-04-5	49
3			Methoxyacetic acid, 3-pentadecyl...	300	C18H36O3	1010282-05-2	49
4			Oxalic acid, allyl decyl ester	270	C15H26O4	1010309-23-8	41
5			Nonadecane	268	C19H40	000629-92-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
Operator : MA/JU
Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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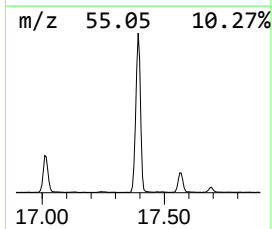
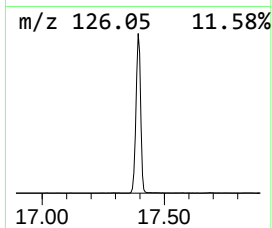
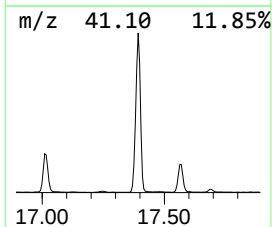
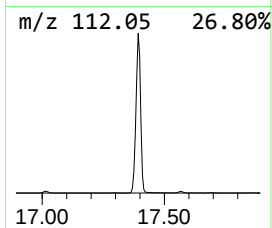
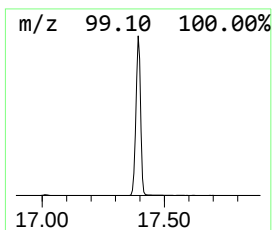
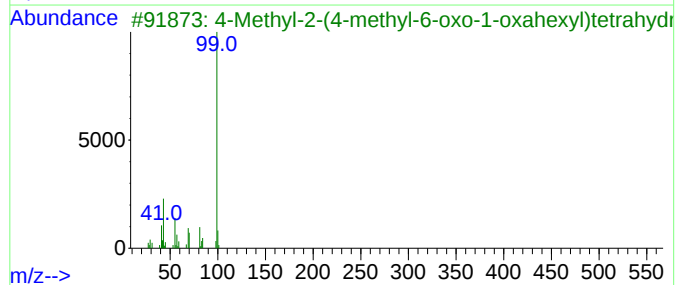
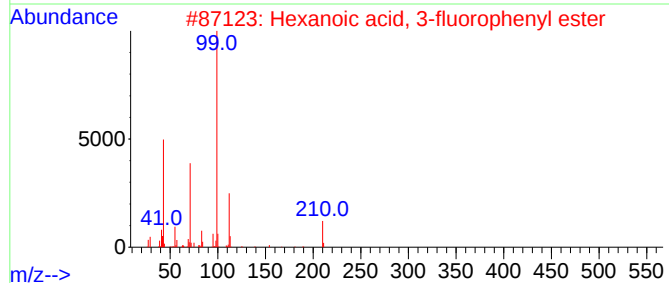
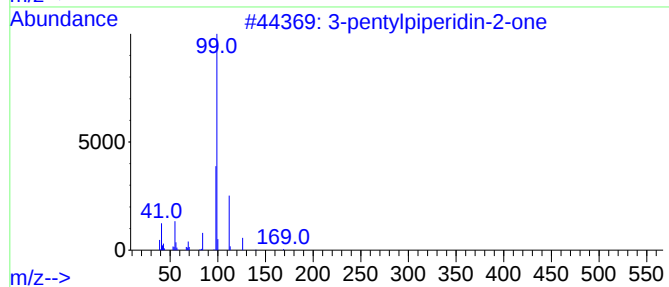
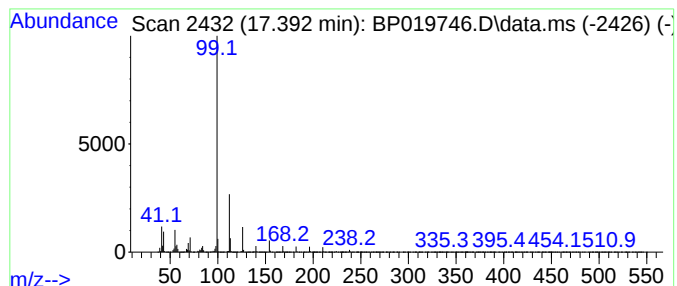
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Hexanoic acid, 3-fluorophen... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.392	232.48 ng	8764740	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-pentylpiperidin-2-one	169	C10H19NO	1000441-61-6	56
2			Hexanoic acid, 3-fluorophenyl ester	210	C12H15FO2	1000330-93-1	50
3			4-Methyl-2-(4-methyl-6-oxo-1-oxa...	214	C12H22O3	101153-83-7	47
4			Phosphonofluoridic acid, methyl-...	210	C9H20FO2P	144313-52-0	47
5			Hexanamide, N-hexanoyl-N-allyl-	253	C15H27NO2	1000340-15-1	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
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Sample : P1440-05
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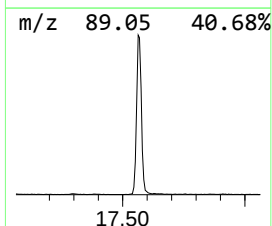
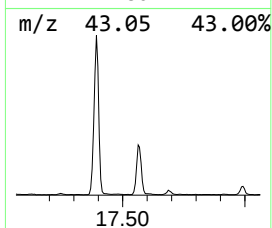
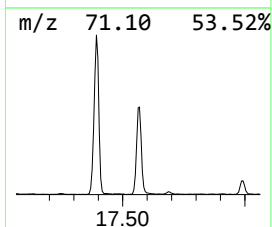
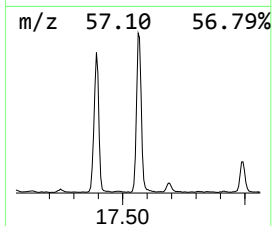
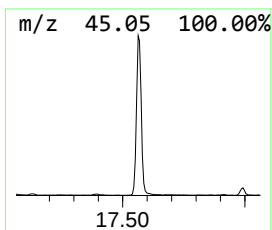
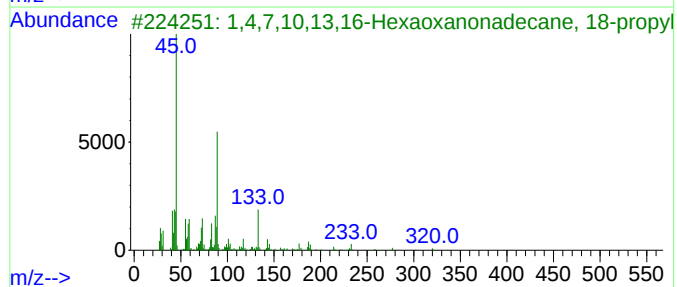
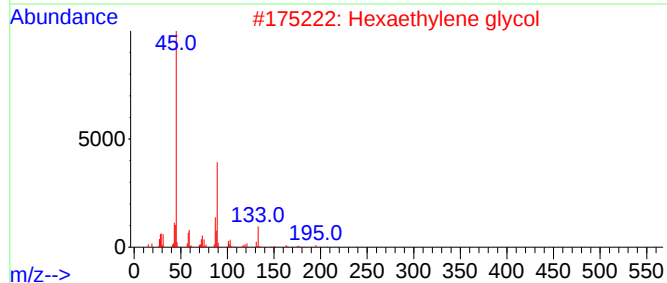
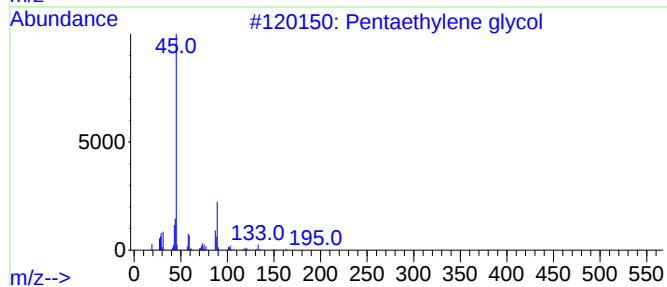
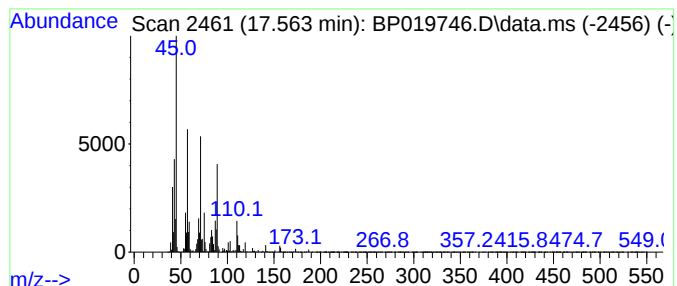
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Pentaethylene glycol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.563	41.57 ng	1567190	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentaethylene glycol	238	C10H22O6	004792-15-8	58
2			Hexaethylene glycol	282	C12H26O7	002615-15-8	58
3			1,4,7,10,13,16-Hexaoxonadecane...	320	C16H32O6	1000163-65-3	53
4			2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	50
5			Heptaethylene glycol	326	C14H30O8	005617-32-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
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Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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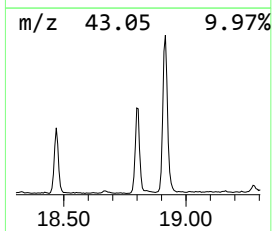
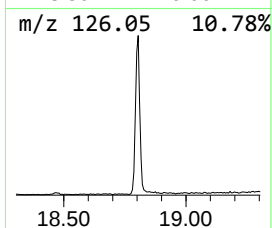
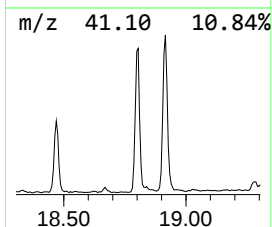
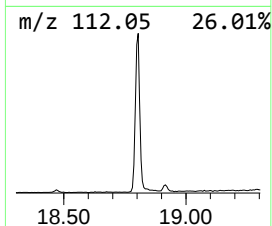
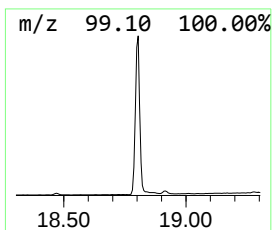
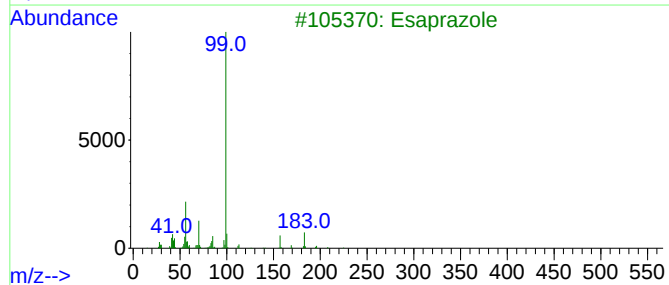
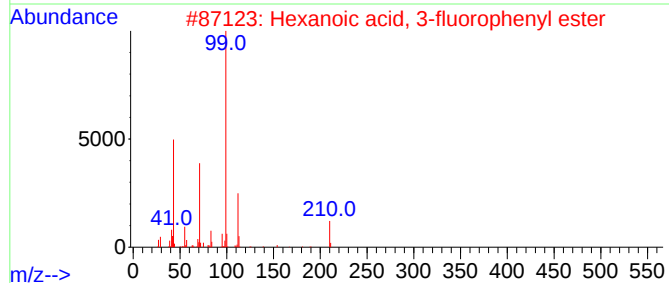
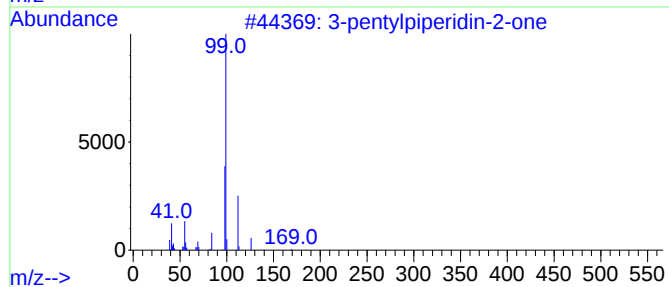
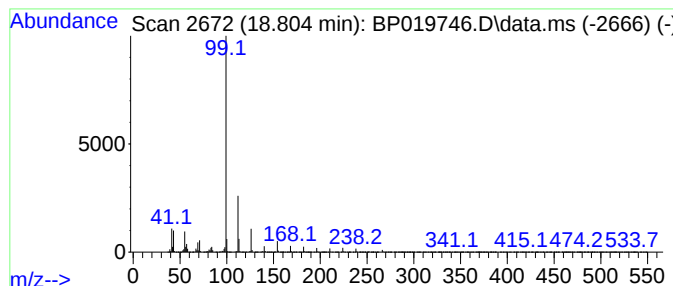
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Esaprazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.804	52.42 ng	1976480	Phenanthrene-d10	17.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-pentylpiperidin-2-one	169	C10H19NO	1000441-61-6	64
2		Hexanoic acid, 3-fluorophenyl ester	210	C12H15FO2	1000330-93-1	50
3		Esaprazole	225	C12H23N3O	064204-55-3	50
4		Hexanoic acid, 2-fluorophenyl ester	210	C12H15FO2	1010325-69-8	45
5		Octanamide, N-allyl-	183	C11H21NO	1000340-16-0	39



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
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Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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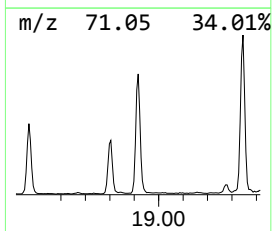
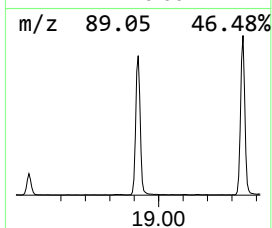
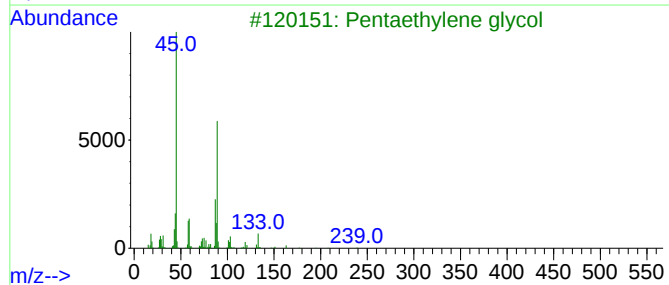
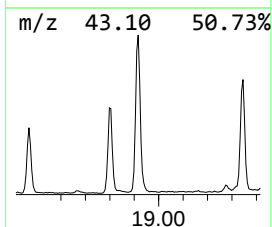
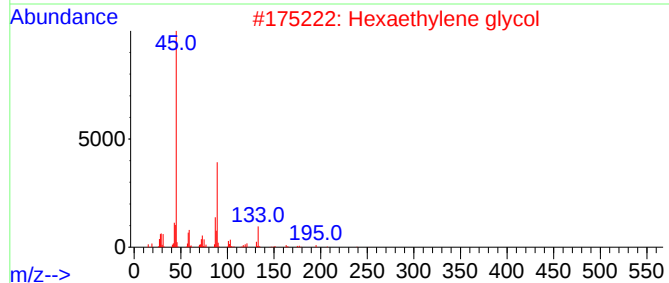
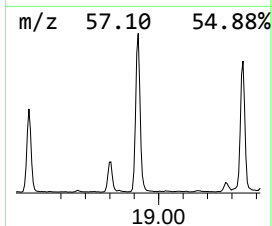
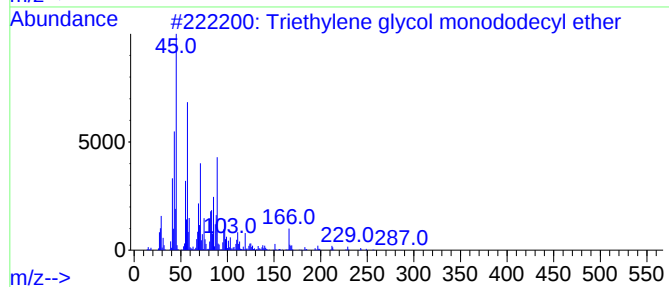
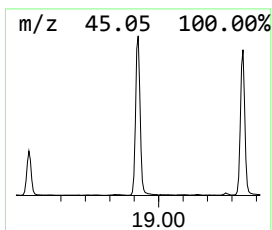
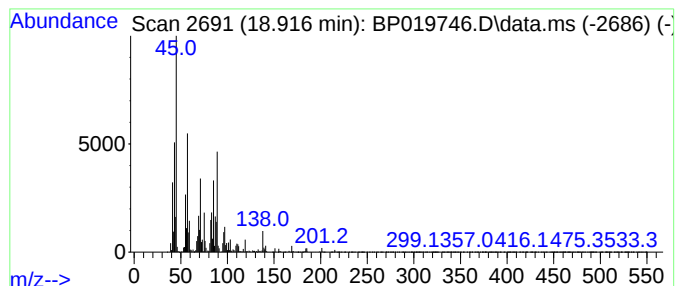
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Triethylene glycol monodode... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.916	56.01 ng	2111690	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	74
2			Hexaethylene glycol	282	C12H26O7	002615-15-8	52
3			Pentaethylene glycol	238	C10H22O6	004792-15-8	50
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
5			Heptaethylene glycol	326	C14H30O8	005617-32-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
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Operator : MA/JU
Sample : P1440-05
Misc :
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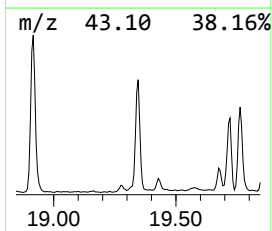
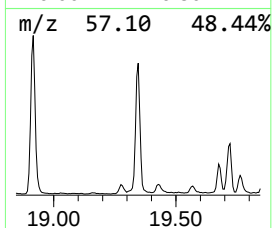
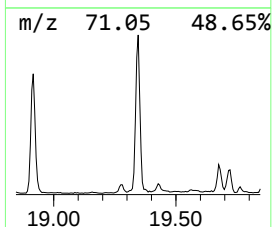
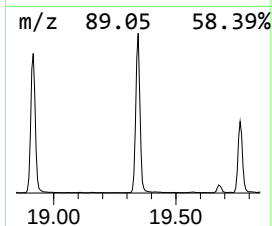
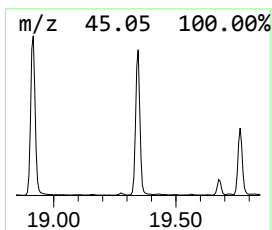
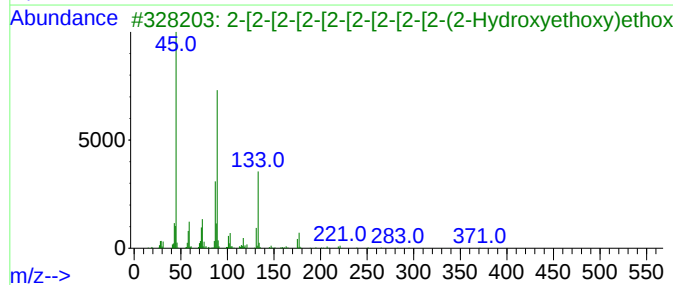
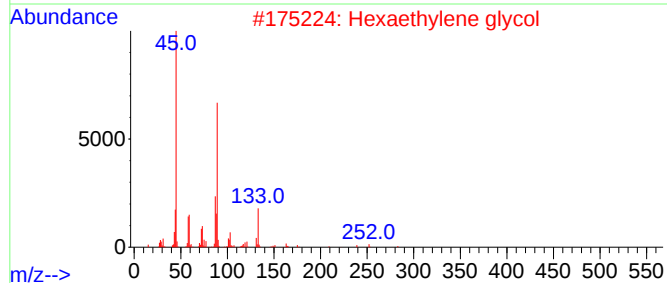
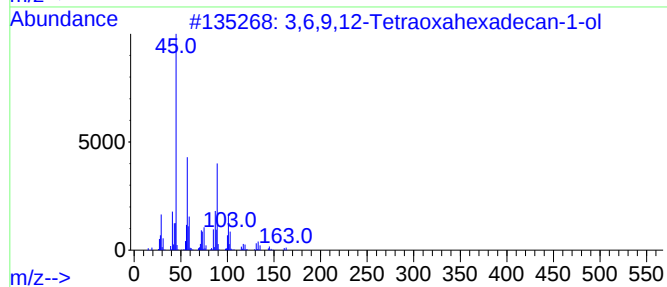
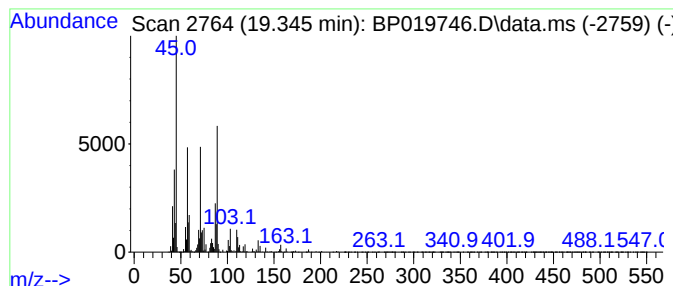
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.345	30.85 ng	1639230	Chrysene-d12		21.386	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxahexadecan-1-ol		250	C12H26O5	001559-34-8	74
2	Hexaethylene glycol		282	C12H26O7	002615-15-8	74
3	2-[2-[2-[2-[2-[2-[2-(2-Hyd...		458	C20H42O11	005579-66-8	72
4	Heptaethylene glycol		326	C14H30O8	005617-32-3	72
5	2-[2-[2-[2-[2-[2-(2-Hydroxyvet...		370	C16H34O9	005117-19-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId :
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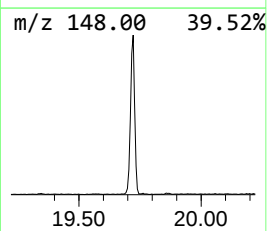
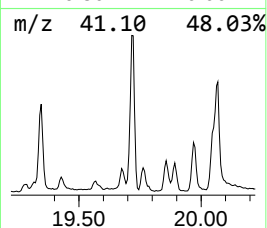
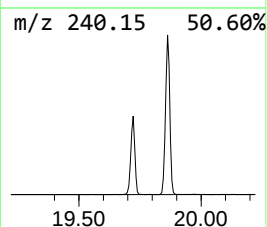
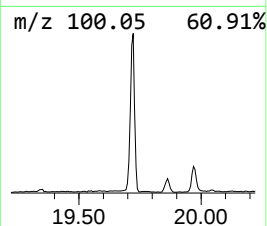
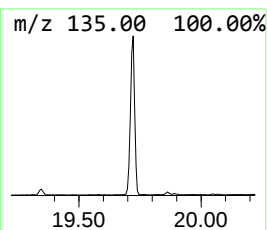
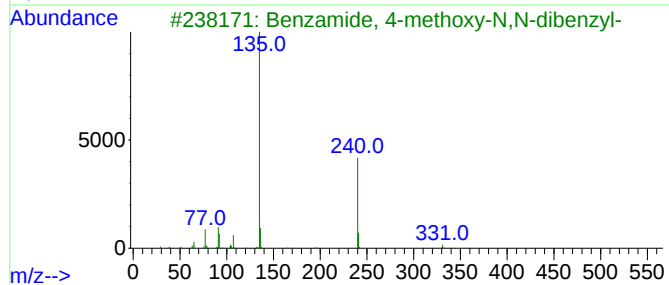
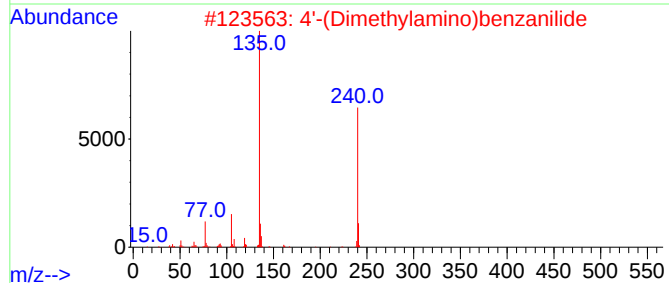
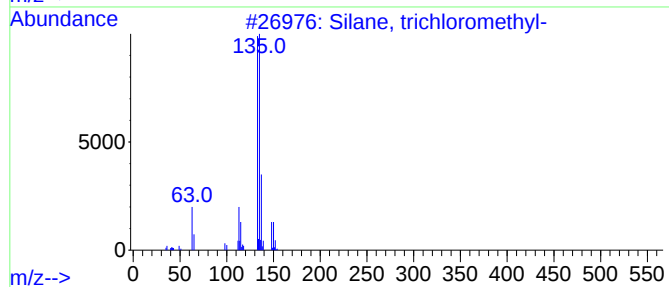
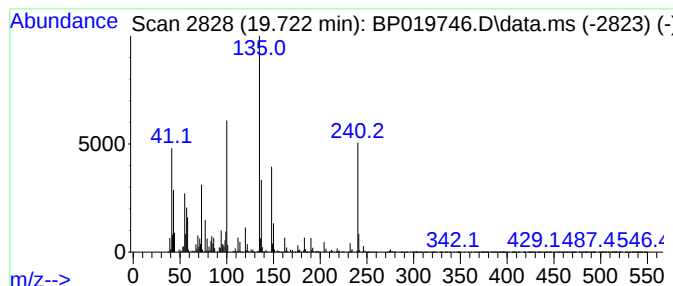
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown19.722 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.722	30.43 ng	1616760	Chrysene-d12	21.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, trichloromethyl-	148	CH3Cl3Si	000075-79-6	38
2			4'-(Dimethylamino)benzanilide	240	C15H16N2O	033986-97-9	25
3			Benzamide, 4-methoxy-N,N-dibenzyl-	331	C22H21NO2	1000451-06-0	25
4			Silane, trimethylphenyl-	150	C9H14Si	000768-32-1	22
5			o-Methoxybenzoic acid, 2-methylp...	242	C15H14O3	072566-70-2	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
Operator : MA/JU
Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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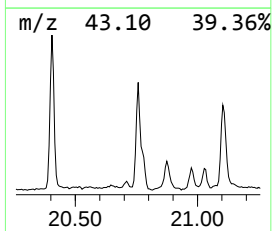
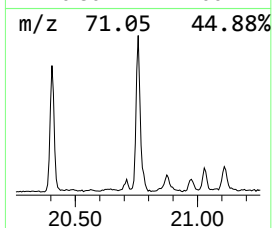
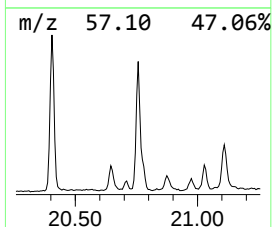
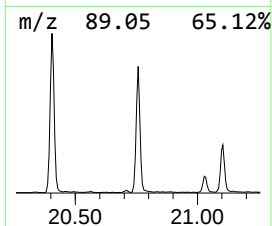
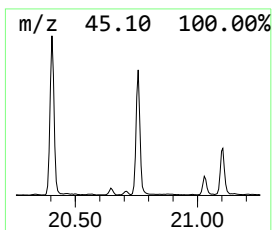
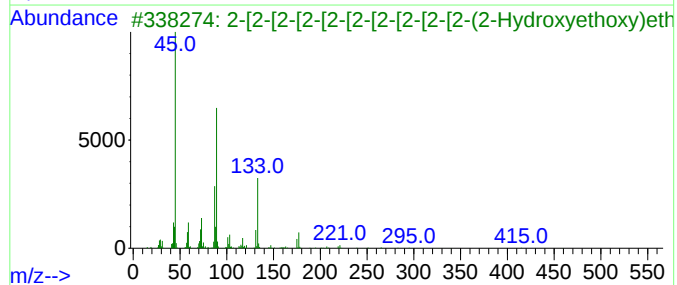
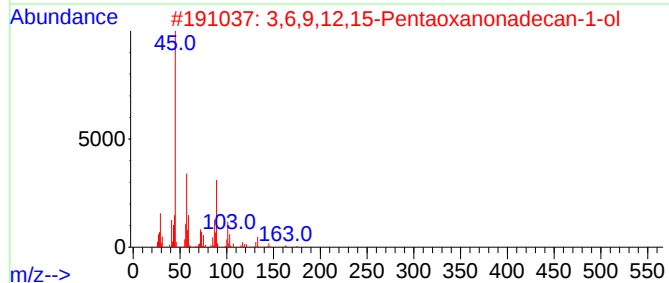
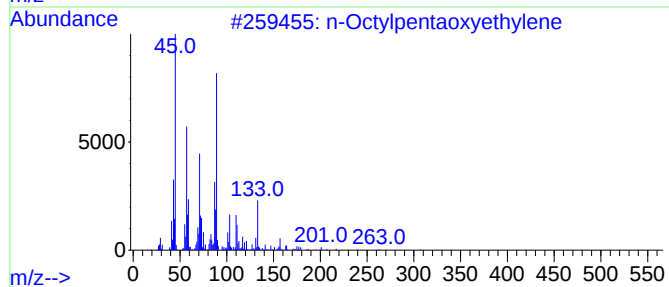
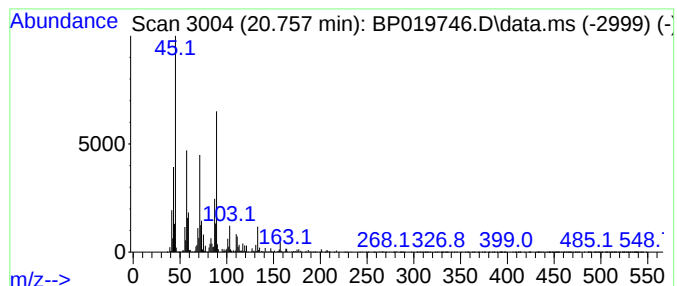
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 n-Octylpentaoxyethylene Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.757	24.91 ng	1323490	Chrysene-d12	21.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Octylpentaoxyethylene	350	C18H38O6	019327-40-3	91
2			3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	74
3			2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	006809-70-7	72
4			2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	005579-66-8	72
5			1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
Operator : MA/JU
Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-3

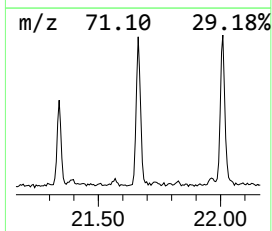
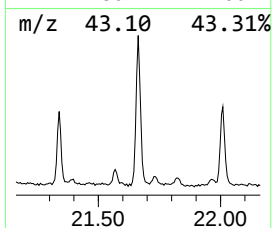
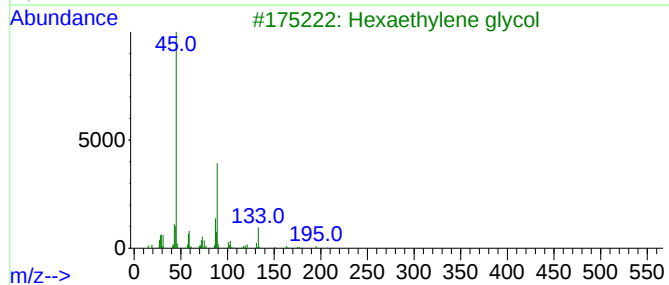
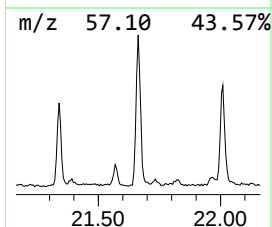
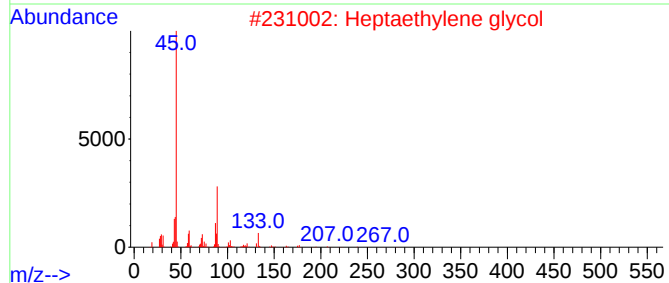
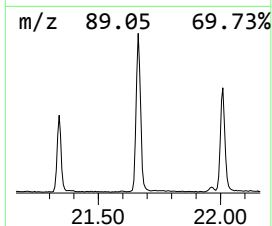
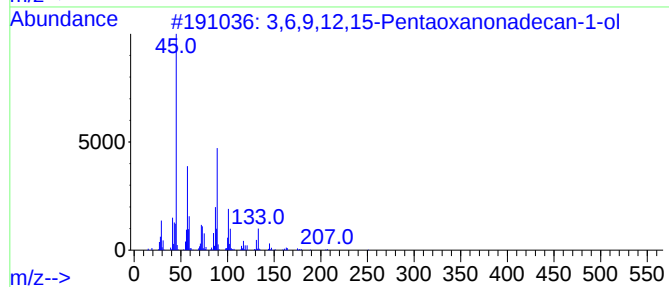
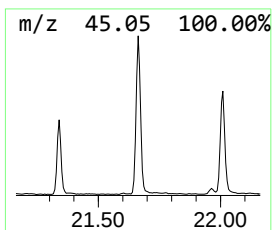
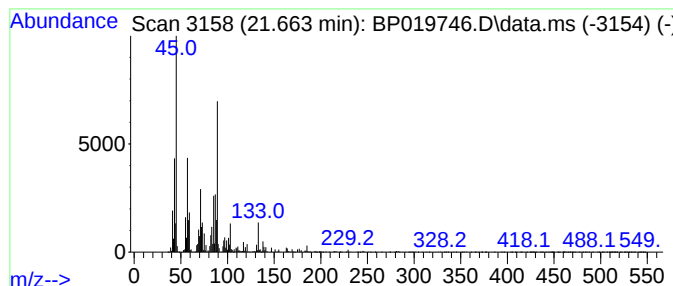
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.663	23.65 ng	1256390	Chrysene-d12	21.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	83	
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	74	
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	74	
4	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	72	
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	64	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019746.D
Acq On : 16 Feb 2024 15:50
Operator : MA/JU
Sample : P1440-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.534	6.534	29.9	ng	641257	1	7.905	429148	20.0
1-Octanol	8.640	49.0	ng	1051220	1	7.905	429148	20.0
1-Decanol	11.740	60.6	ng	1586770	2	10.699	523760	20.0
unknown12.263	12.263	36.4	ng	954105	2	10.699	523760	20.0
3-pentylpiperid...	13.675	60.5	ng	1886720	3	14.534	624268	20.0
1-Decene	14.187	26.5	ng	827905	3	14.534	624268	20.0
unknown14.593	14.593	41.9	ng	1309130	3	14.534	624268	20.0
Dodecanoic acid	14.993	35.3	ng	1101380	3	14.534	624268	20.0
unknown15.298	15.298	46.4	ng	1448460	3	14.534	624268	20.0
Octadecane, 1-i...	15.710	44.9	ng	1401140	3	14.534	624268	20.0
Diethylene glyc...	17.010	46.4	ng	1750570	4	17.292	754021	20.0
Hexanoic acid, ...	17.392	232.5	ng	8764740	4	17.292	754021	20.0
Pentaethylene g...	17.563	41.6	ng	1567190	4	17.292	754021	20.0
Esaprazole	18.804	52.4	ng	1976480	4	17.292	754021	20.0
Triethylene gly...	18.916	56.0	ng	2111690	4	17.292	754021	20.0
3,6,9,12-Tetrao...	19.345	30.9	ng	1639230	5	21.386	1062670	20.0
unknown19.722	19.722	30.4	ng	1616760	5	21.386	1062670	20.0
2-[2-[2-[2-[2-...	20.404	34.0	ng	1808610	5	21.386	1062670	20.0
n-Octylpentaoxy...	20.757	24.9	ng	1323490	5	21.386	1062670	20.0
3,6,9,12,15-Pen...	21.663	23.6	ng	1256390	5	21.386	1062670	20.0