

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080824\
 Data File : BF138876.D
 Acq On : 08 Aug 2024 20:34
 Operator : RC/JU
 Sample : P3483-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A

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_F\Methods\8270-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138876.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	6	16	rVB	451946	670678	70.29%	8.000%
2	2.240	20	25	33	rVB	6481	10541	1.10%	0.126%
3	3.393	216	221	227	rBV	8053	21958	2.30%	0.262%
4	5.063	500	505	520	rVB	73504	111555	11.69%	1.331%
5	5.475	569	575	591	rBV	692521	927381	97.19%	11.062%
6	6.481	741	746	763	rBV	695426	954201	100.00%	11.382%
7	6.675	773	779	791	rBV	16323	26673	2.80%	0.318%
8	6.840	802	807	812	rBV	212288	255254	26.75%	3.045%
9	7.404	897	903	908	rBV	473016	601932	63.08%	7.180%
10	7.657	941	946	953	rVB	12355	15935	1.67%	0.190%
11	8.116	1019	1024	1038	rVB	244380	314157	32.92%	3.747%
12	8.340	1058	1062	1067	rBB	8661	10342	1.08%	0.123%
13	8.434	1074	1078	1092	rBV	56347	81522	8.54%	0.972%
14	9.192	1201	1207	1212	rBV	760186	924979	96.94%	11.034%
15	9.586	1270	1274	1279	rVB	30723	37234	3.90%	0.444%
16	9.869	1317	1322	1327	rBV	237264	294895	30.90%	3.518%
17	9.963	1332	1338	1345	rBV	30251	45982	4.82%	0.548%
18	10.663	1452	1457	1472	rBV	336131	439000	46.01%	5.237%
19	11.357	1570	1575	1585	rBV2	194090	287177	30.10%	3.426%
20	11.433	1585	1588	1592	rVB	9364	10763	1.13%	0.128%
21	11.757	1637	1643	1648	rVB2	26364	40439	4.24%	0.482%
22	11.886	1657	1665	1671	rBV3	33682	62339	6.53%	0.744%
23	11.969	1676	1679	1687	rVB2	13341	24870	2.61%	0.297%
24	12.404	1749	1753	1756	rBV	8746	12126	1.27%	0.145%
25	12.569	1776	1781	1786	rBV	112568	139926	14.66%	1.669%
26	12.798	1814	1820	1827	rBV	99056	150807	15.80%	1.799%
27	12.939	1838	1844	1852	rVB	499776	644824	67.58%	7.692%
28	13.010	1853	1856	1862	rBV3	8970	17024	1.78%	0.203%
29	13.127	1869	1876	1879	rBV	15215	29134	3.05%	0.348%
30	13.233	1890	1894	1900	rVB3	10075	14189	1.49%	0.169%
31	13.322	1906	1909	1912	rBV	6746	9859	1.03%	0.118%
32	13.639	1960	1963	1967	rVB	9844	12266	1.29%	0.146%
33	13.745	1978	1981	1983	rBV	12144	15802	1.66%	0.188%
34	13.839	1992	1997	2006	rVB5	40163	90457	9.48%	1.079%
35	13.992	2018	2023	2035	rVB2	199175	378683	39.69%	4.517%
36	14.451	2098	2101	2103	rBV	15306	23078	2.42%	0.275%

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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_F\Methods\8270-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.033	2196	2200	2204	rBV	53087	97824	10.25%	1.167%
38	15.080	2205	2208	2213	rVB	62318	86707	9.09%	1.034%
39	15.333	2248	2251	2256	rVB	24121	33568	3.52%	0.400%
40	15.398	2258	2262	2267	rVV	33810	51037	5.35%	0.609%
41	15.457	2267	2272	2284	rVB	106380	181234	18.99%	2.162%
42	15.880	2340	2344	2351	rVB	46079	78594	8.24%	0.938%
43	16.927	2518	2522	2533	rVB3	18922	49064	5.14%	0.585%
44	17.498	2613	2619	2633	rVB10	27394	97329	10.20%	1.161%

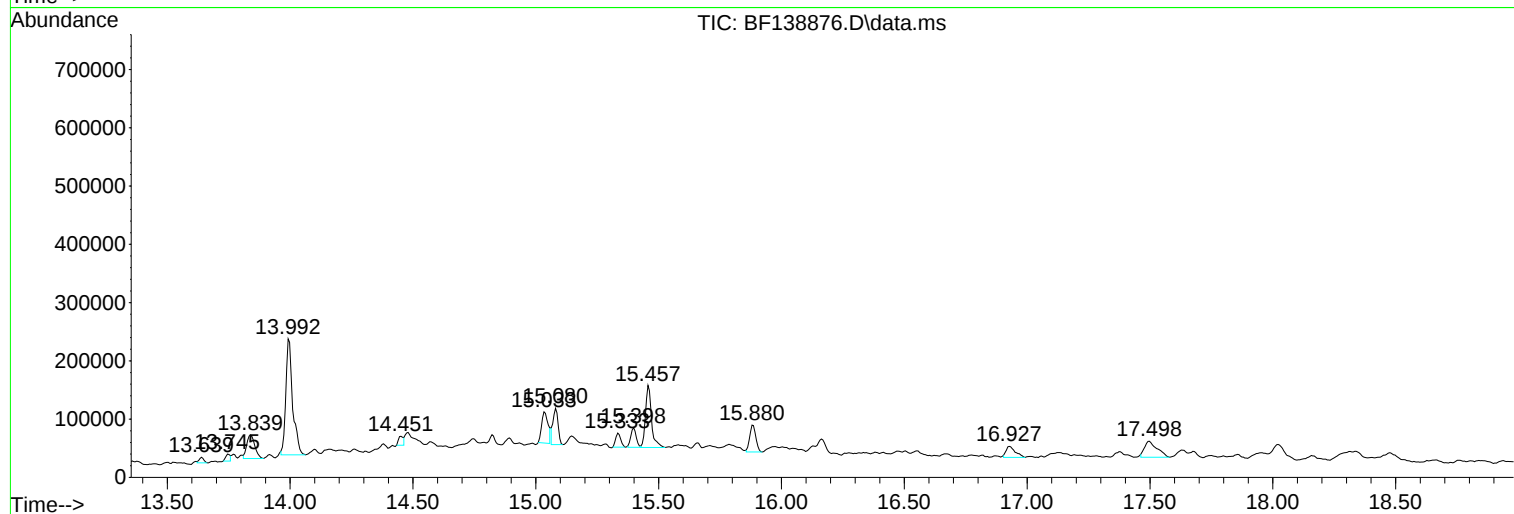
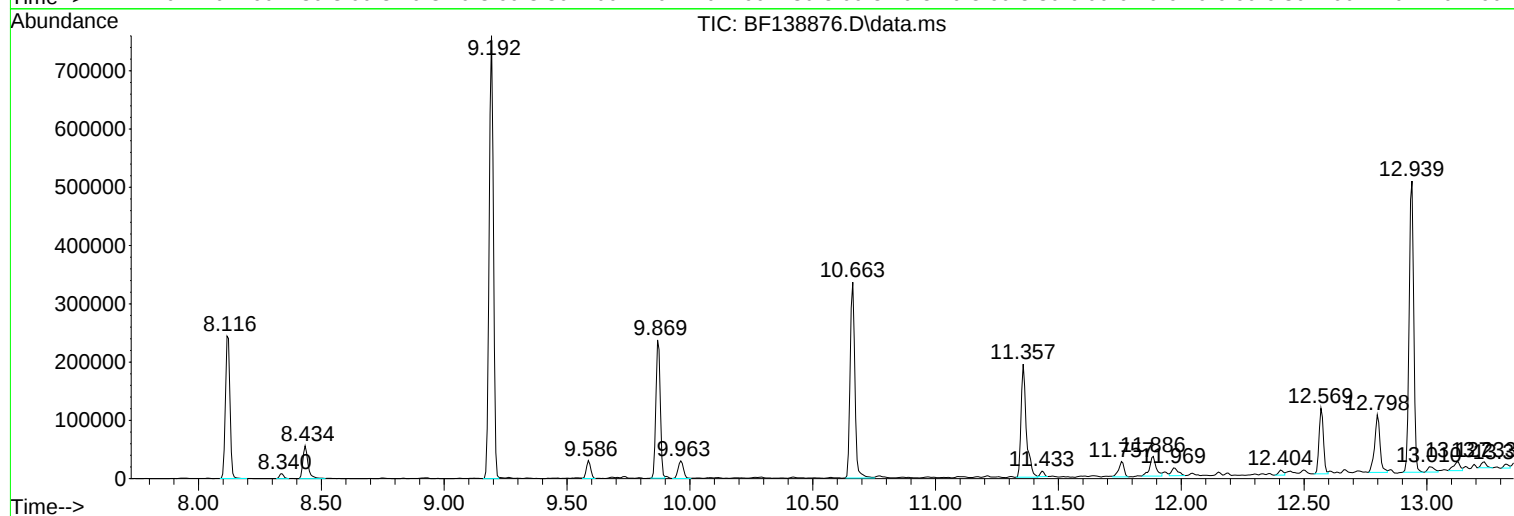
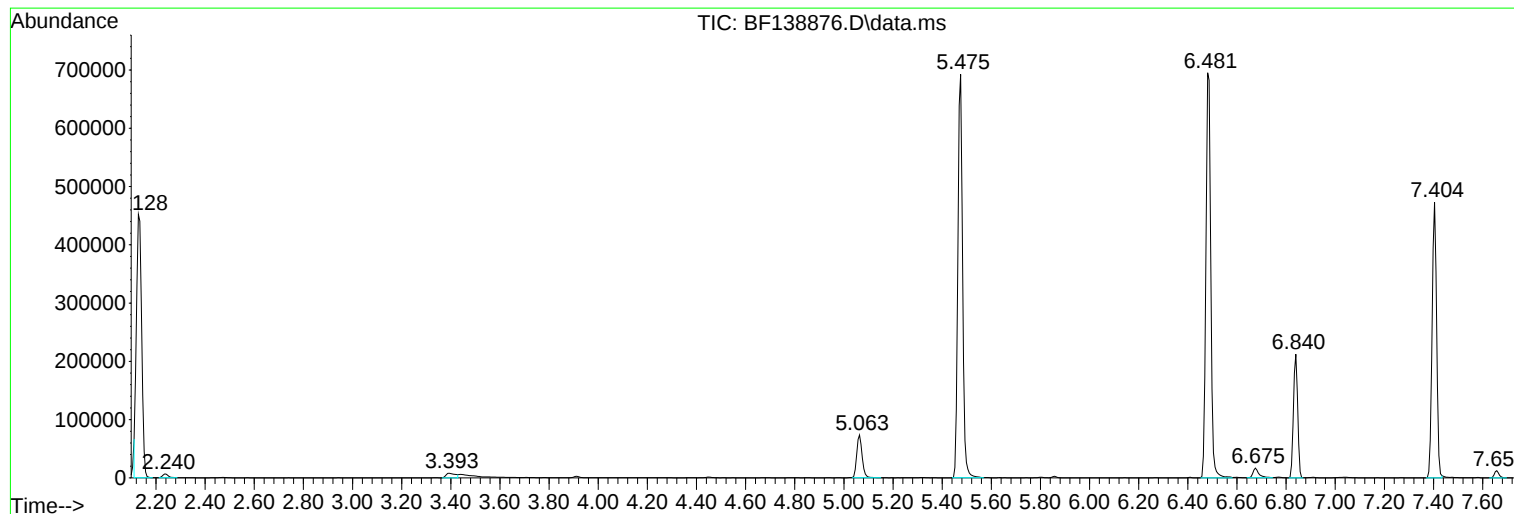
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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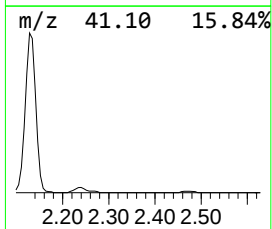
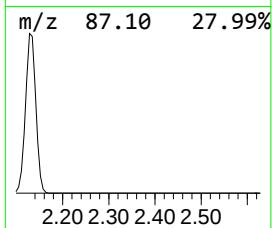
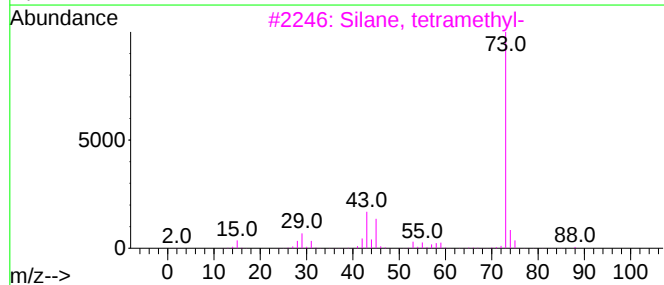
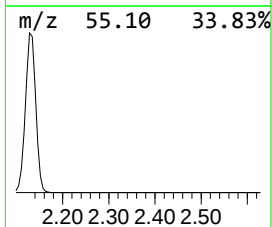
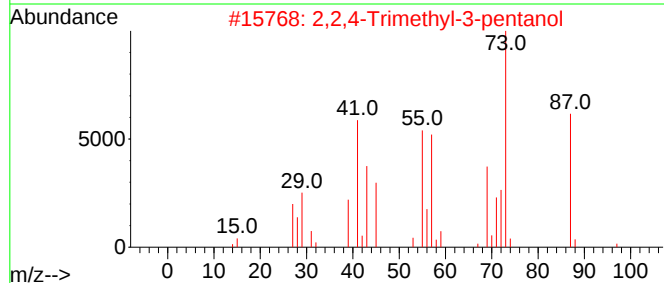
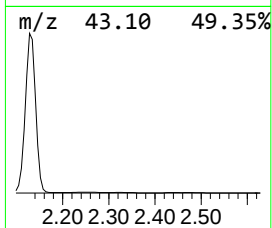
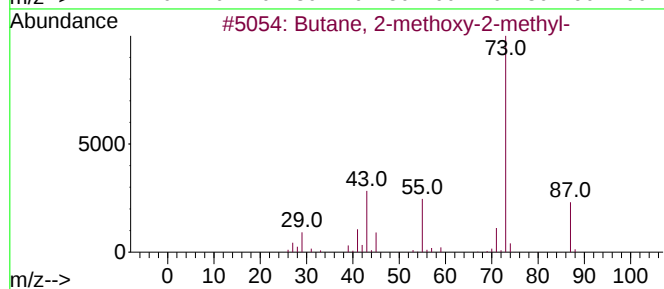
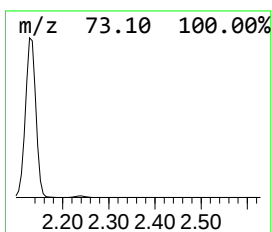
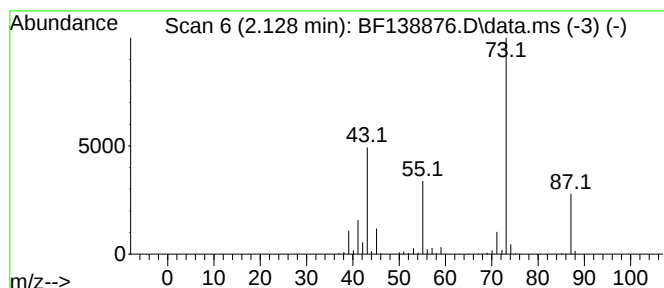
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	52.55 ng	670678	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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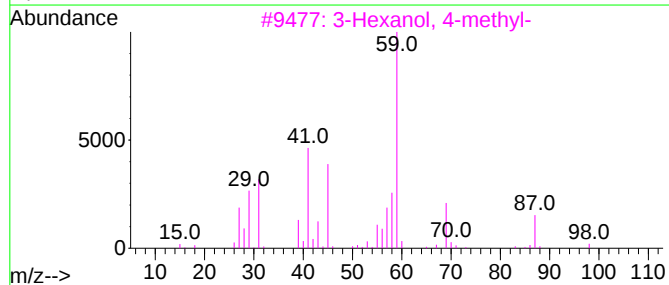
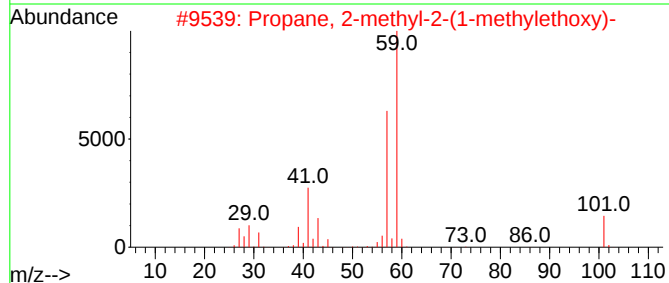
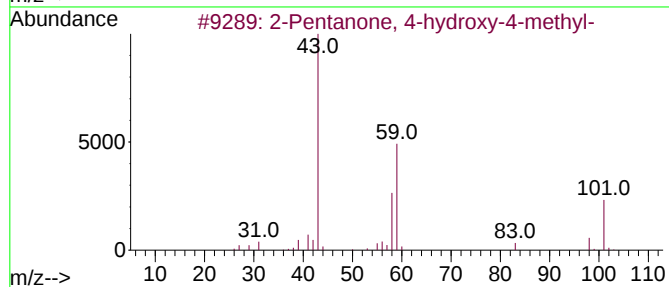
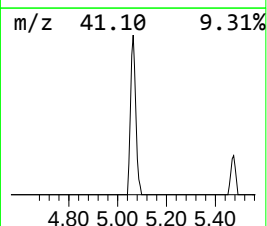
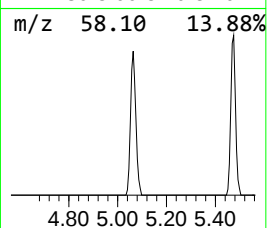
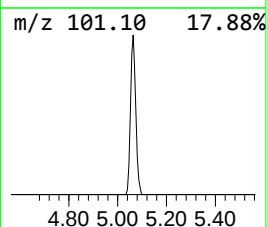
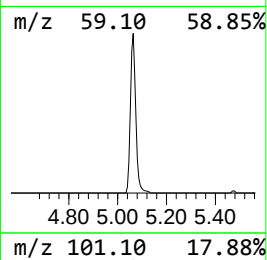
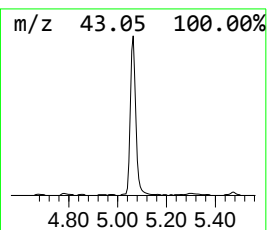
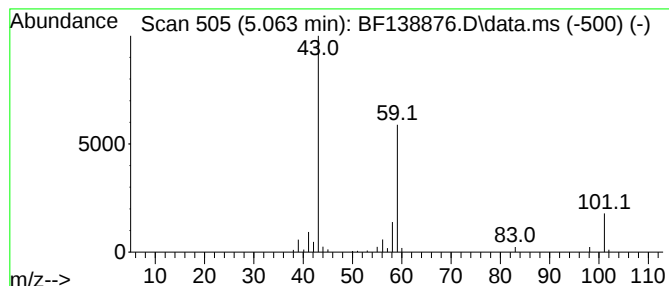
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	8.74 ng	111555	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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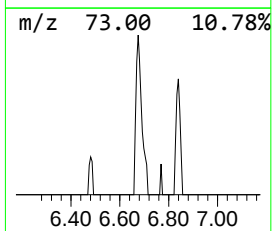
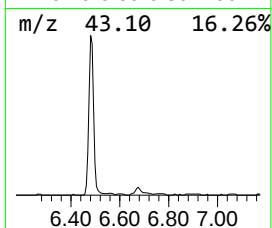
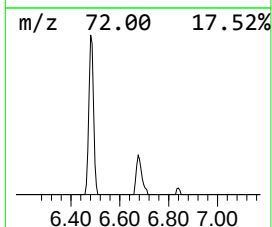
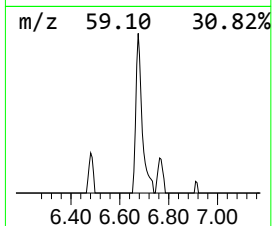
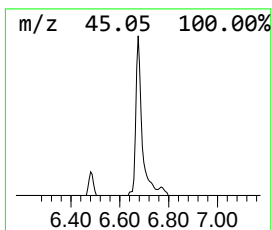
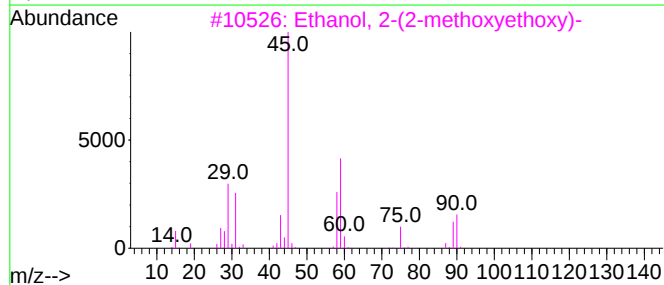
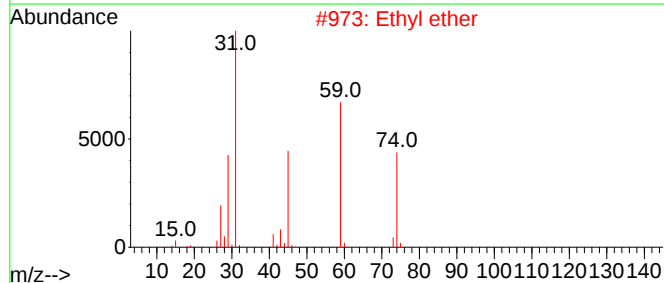
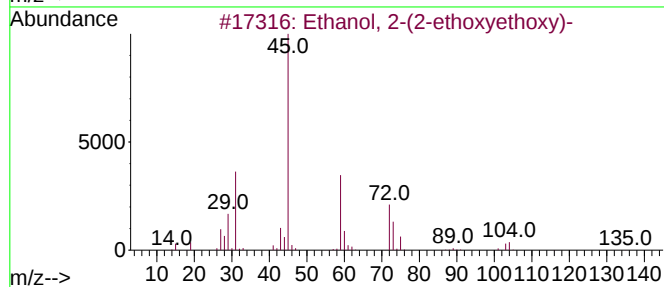
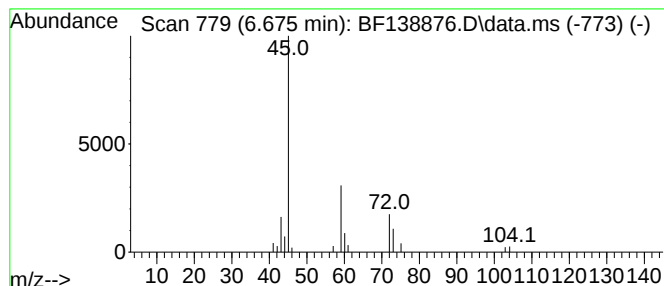
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.675	2.09 ng	26673	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethyl ether	74	C4H10O	000060-29-7	42
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	39
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	38



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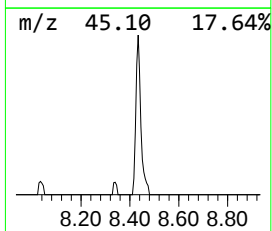
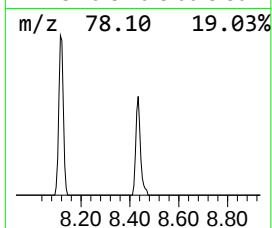
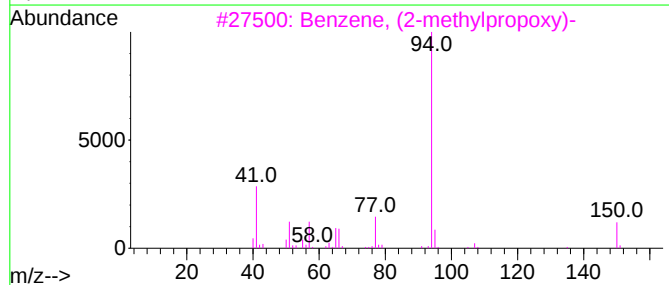
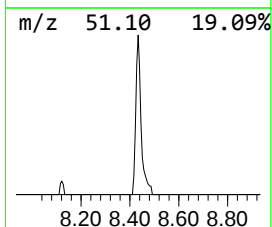
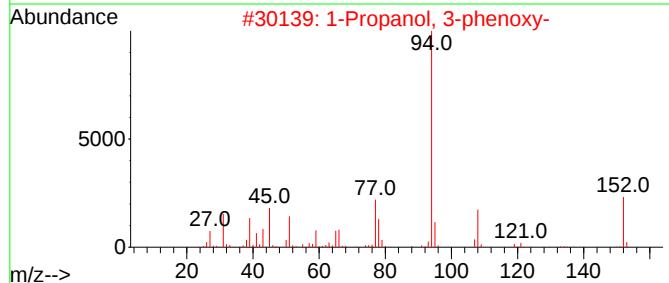
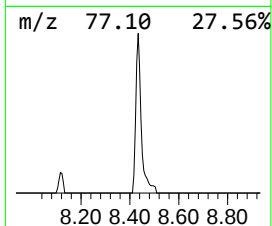
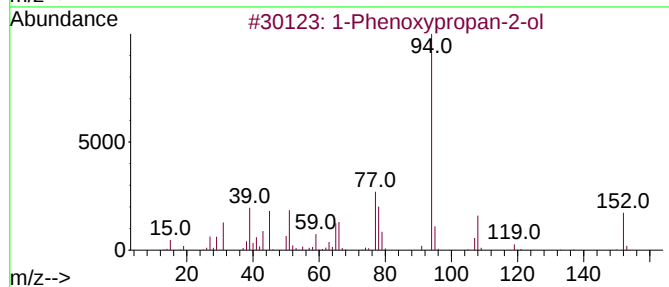
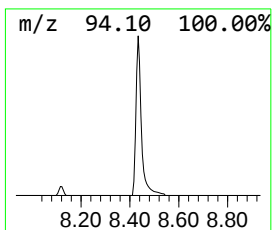
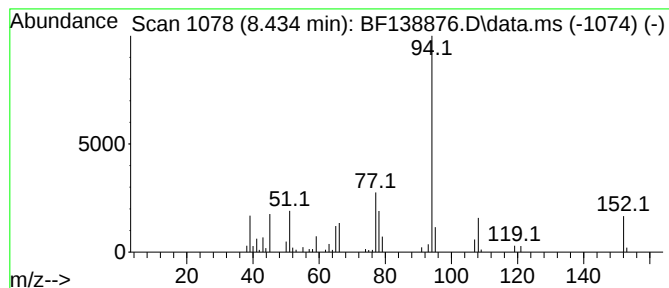
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	5.19 ng	81522	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	59
4			2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	50



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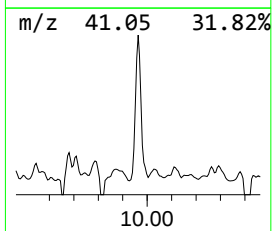
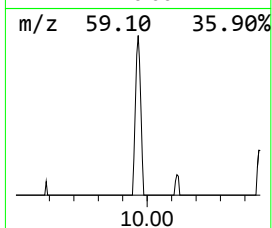
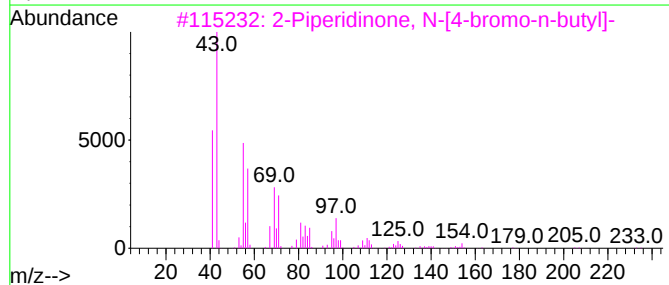
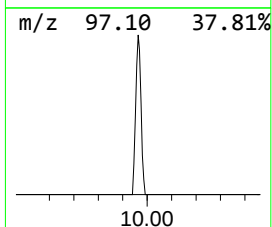
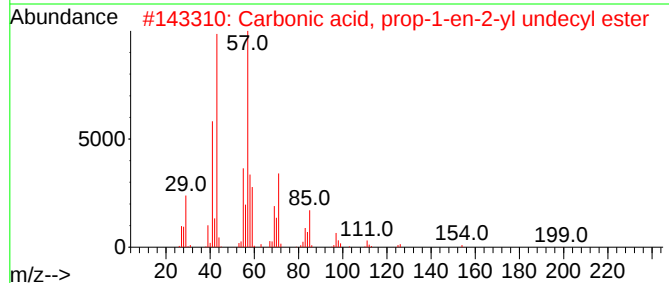
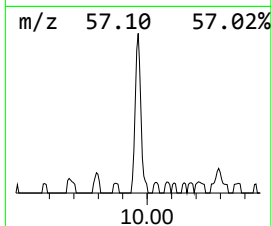
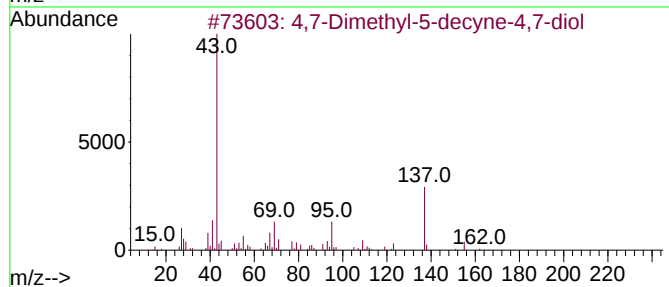
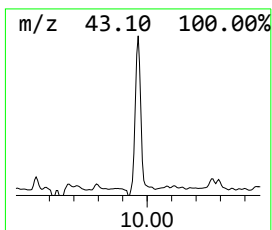
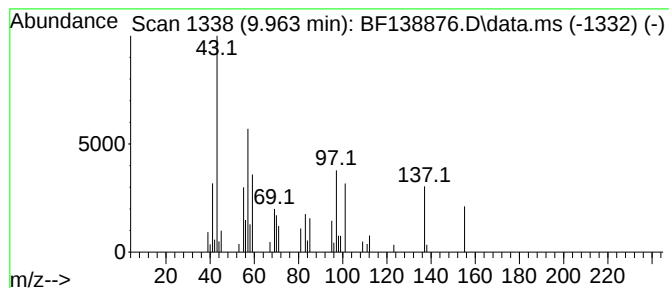
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.963 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.963	3.12 ng	45982	Acenaphthene-d10	9.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	22
2		Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	10
3		2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	10
4		Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	10
5		Dodecyl heptyl ether	284	C19H40O	1010406-39-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080824\
Data File : BF138876.D
Acq On : 08 Aug 2024 20:34
Operator : RC/JU
Sample : P3483-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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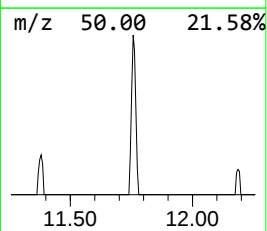
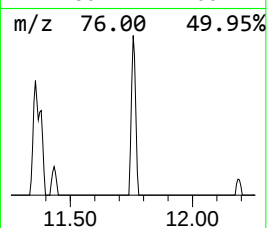
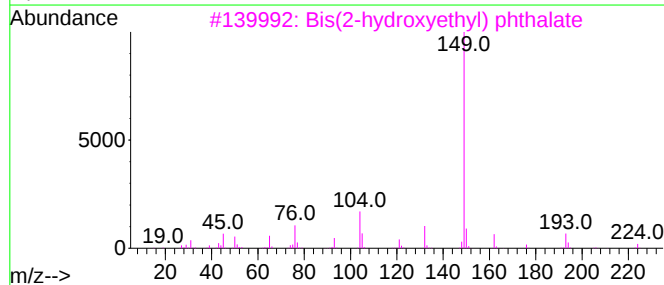
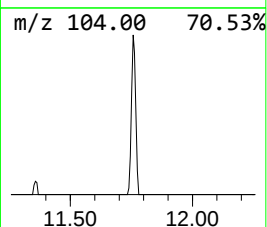
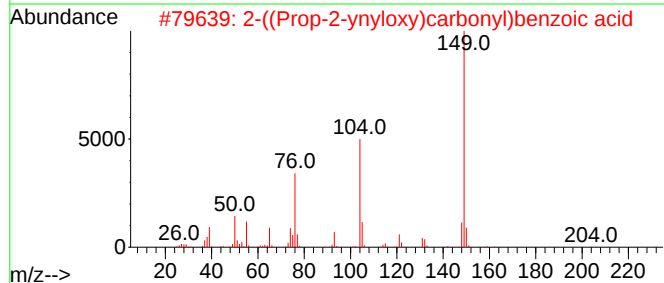
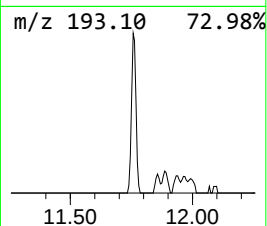
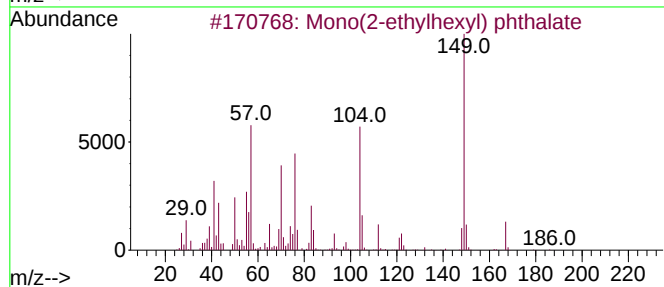
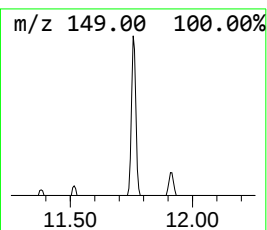
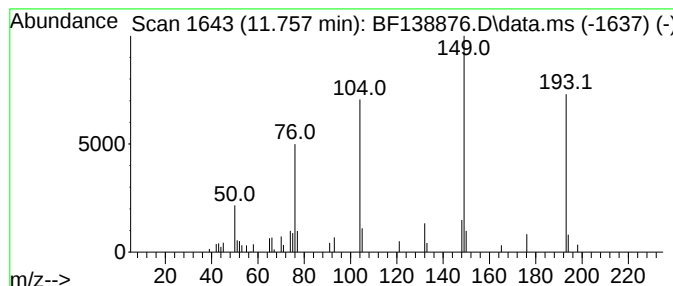
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown11.757 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.757	2.82 ng	40439	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mono(2-ethylhexyl) phthalate	278	C16H22O4	004376-20-9	45
2			2-((Prop-2-ynyloxy)carbonyl)benz...	204	C11H8O4	006139-61-3	45
3			Bis(2-hydroxyethyl) phthalate	254	C12H14O6	000084-73-1	38
4			Diethyl Phthalate	222	C12H14O4	000084-66-2	27
5			6-Amino-1-methylpurine	149	C6H7N5	005142-22-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080824\
Data File : BF138876.D
Acq On : 08 Aug 2024 20:34
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Sample : P3483-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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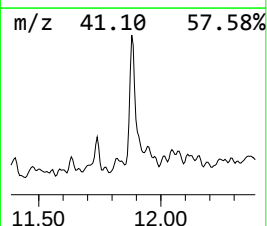
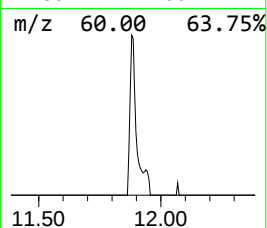
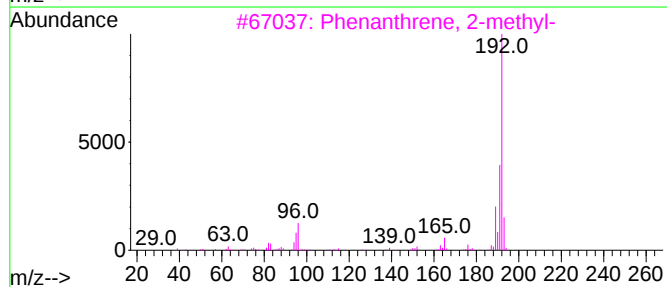
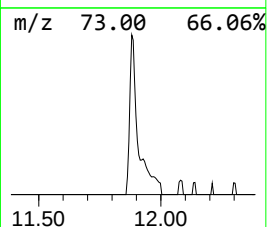
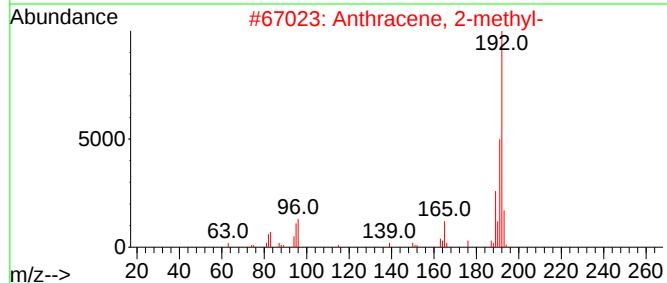
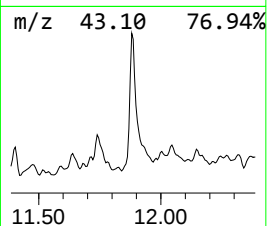
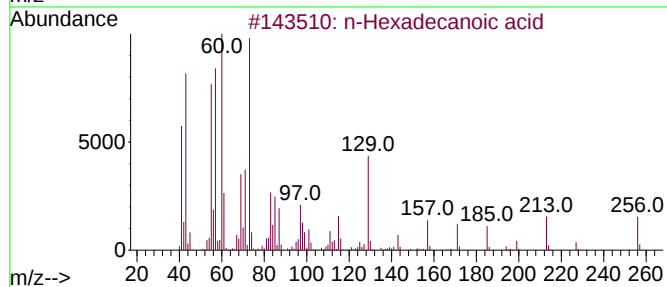
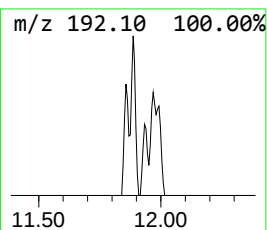
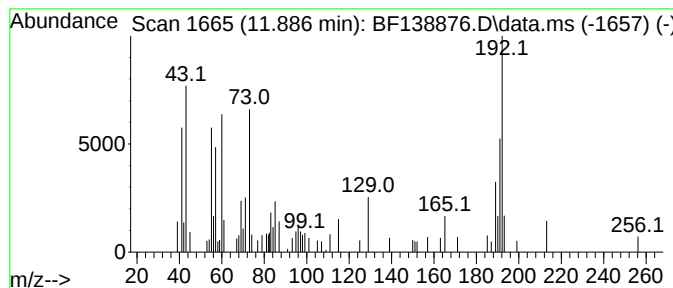
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	4.34 ng	62339	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	64
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	55
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080824\
Data File : BF138876.D
Acq On : 08 Aug 2024 20:34
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Sample : P3483-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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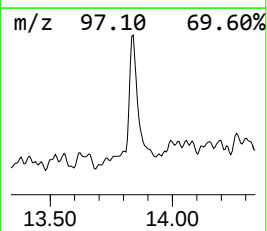
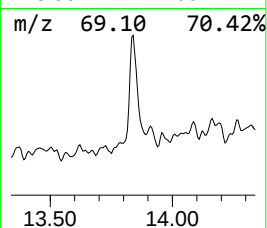
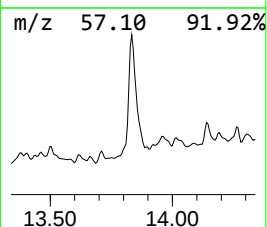
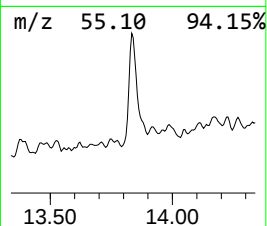
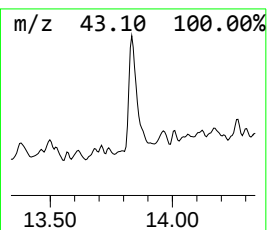
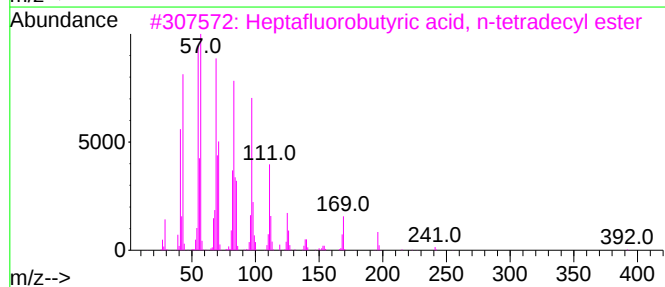
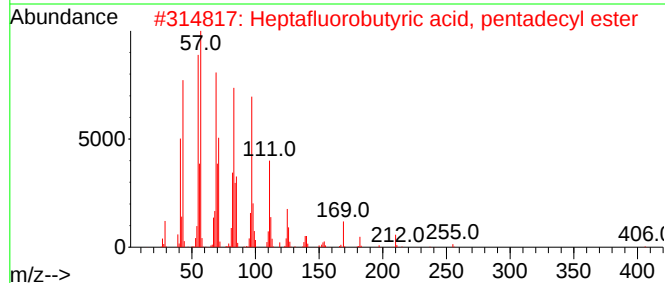
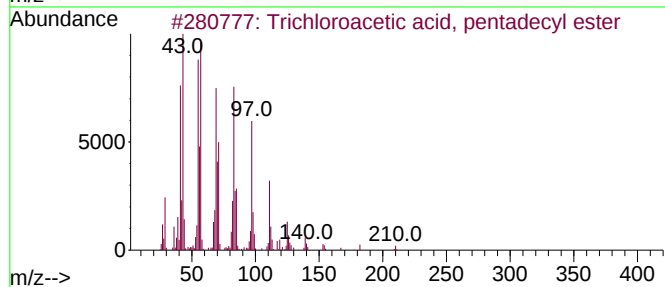
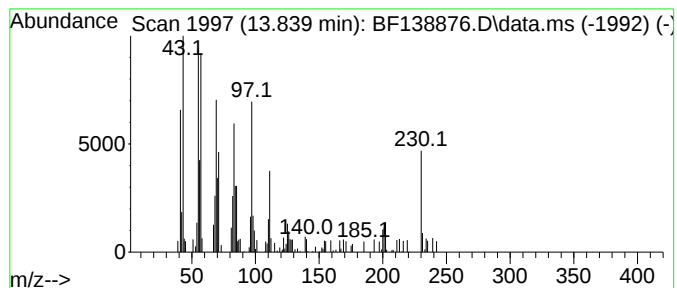
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	4.78 ng	90457	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
3			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
4			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080824\
Data File : BF138876.D
Acq On : 08 Aug 2024 20:34
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Sample : P3483-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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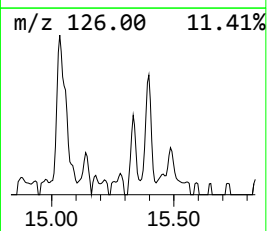
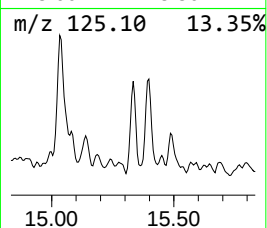
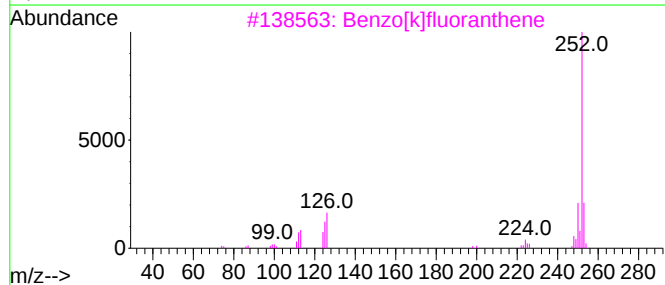
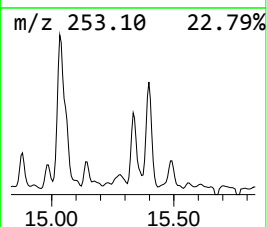
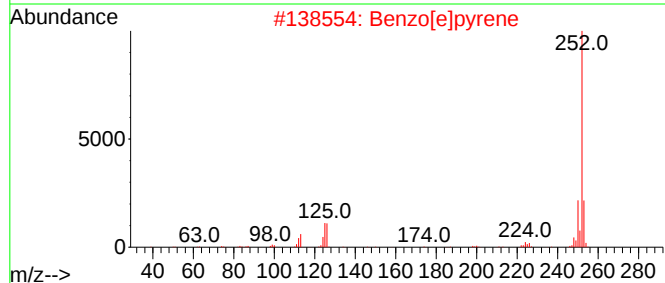
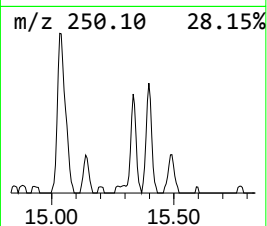
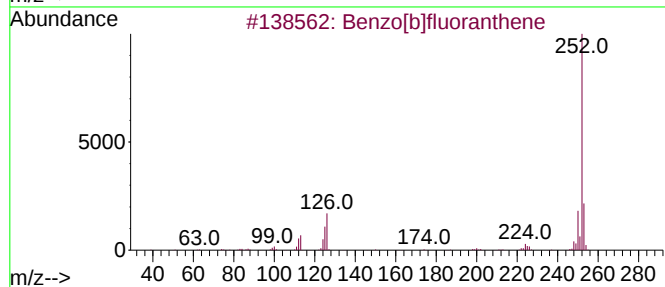
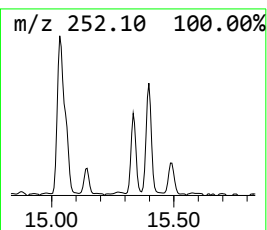
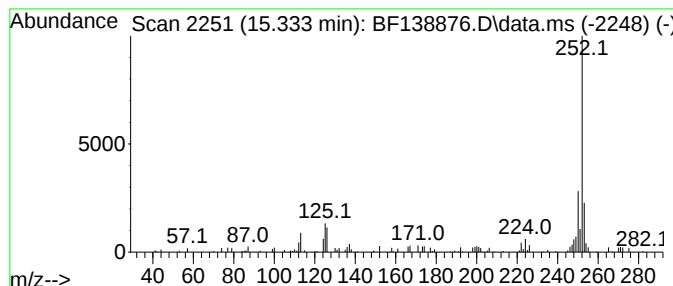
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	3.70 ng	33568	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
2			Benzo[e]pyrene	252	C20H12	000192-97-2	89
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
4			Perylene	252	C20H12	000198-55-0	81
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080824\
Data File : BF138876.D
Acq On : 08 Aug 2024 20:34
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Sample : P3483-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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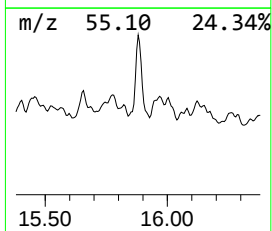
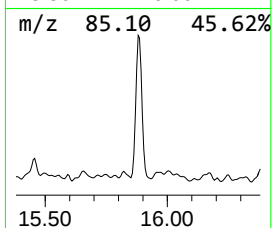
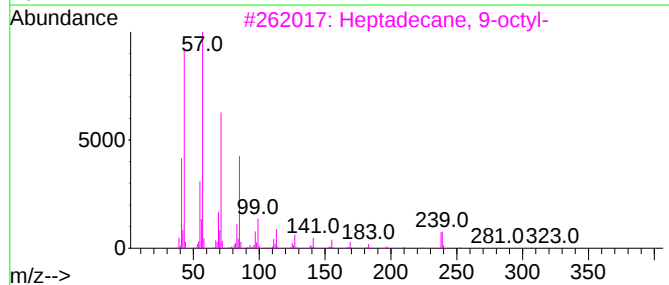
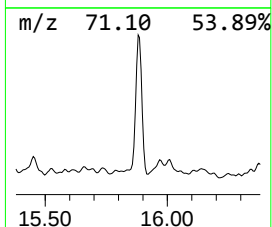
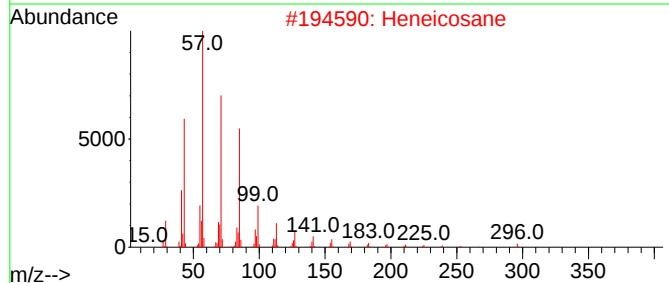
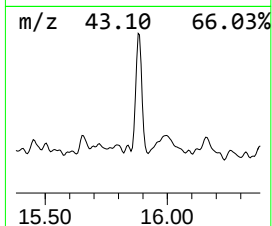
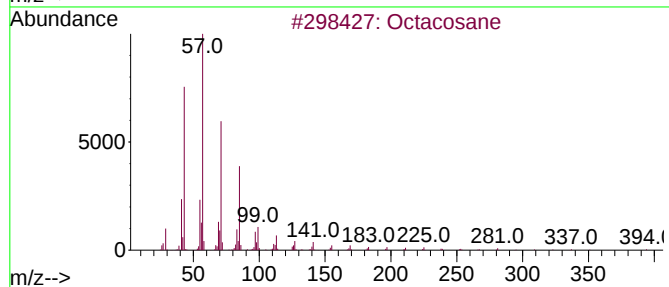
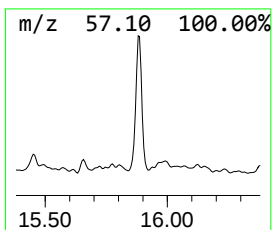
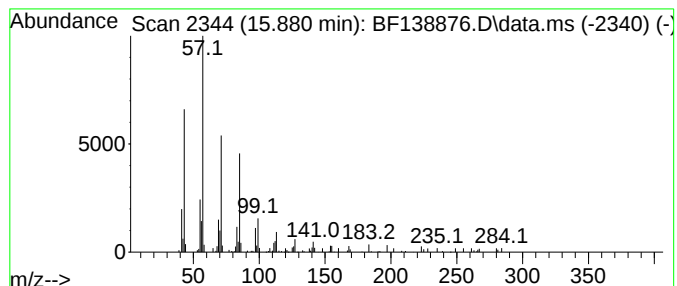
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	8.67 ng	78594	Perylene-d12	15.457

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5		Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080824\
Data File : BF138876.D
Acq On : 08 Aug 2024 20:34
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Sample : P3483-01
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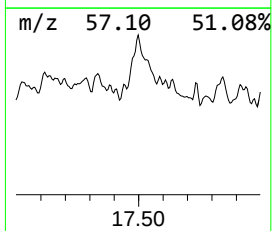
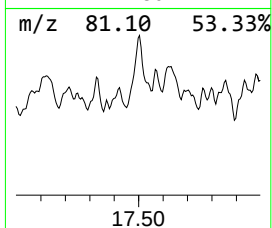
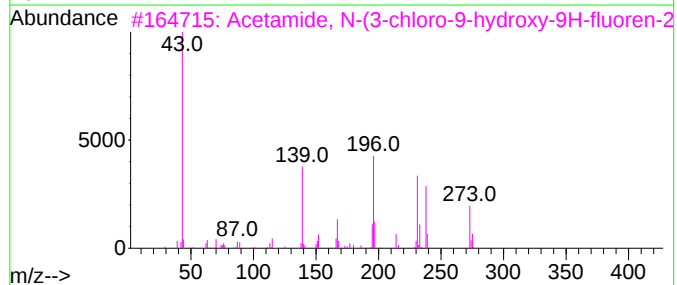
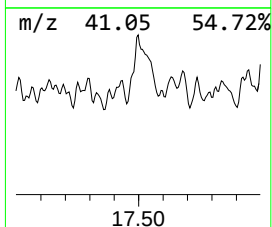
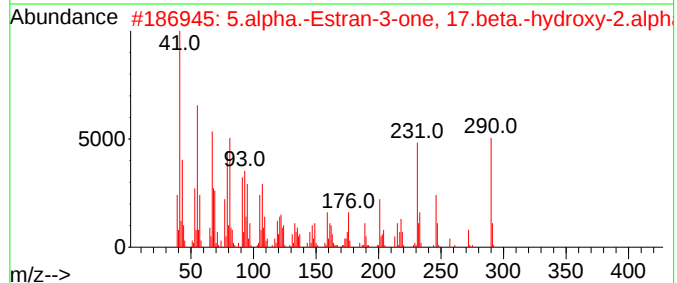
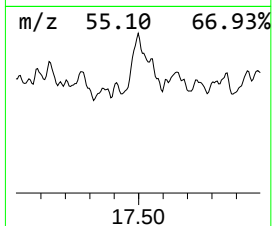
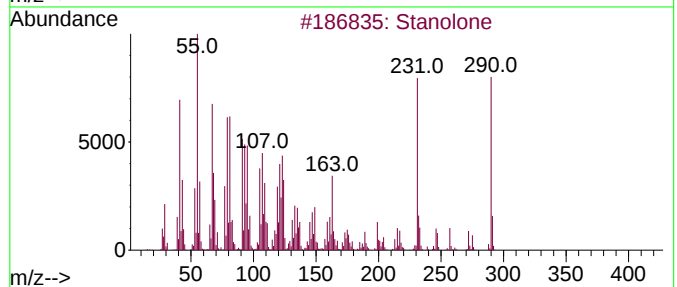
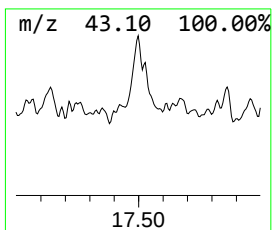
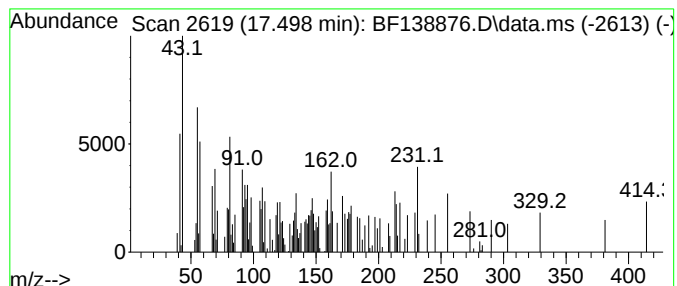
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.498 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.498	10.74 ng	97329	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Stanolone	290	C19H30O2	000521-18-6	45
2			5.alpha.-Estran-3-one, 17.beta.-...	290	C19H30O2	004267-75-8	18
3			Acetamide, N-(3-chloro-9-hydroxy...	273	C15H12ClNO2	1000305-19-1	12
4			Ethanone, 1-(1,2,3,4,7,7a-hexahy...	246	C17H26O	032388-58-2	10
5			Succinic acid, hex-4-yn-3-yl 2,3...	328	C16H15F3O4	1010390-76-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080824\
Data File : BF138876.D
Acq On : 08 Aug 2024 20:34
Operator : RC/JU
Sample : P3483-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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
Butane, 2-metho...	2.128	52.5	ng	670678	1	6.840	255254	20.0
2-Pentanone, 4-...	5.063	8.7	ng	111555	1	6.840	255254	20.0
Ethanol, 2-(2-e...	6.675	2.1	ng	26673	1	6.840	255254	20.0
1-Phenoxypropan...	8.434	5.2	ng	81522	2	8.122	314157	20.0
unknown9.963	9.963	3.1	ng	45982	3	9.869	294895	20.0
unknown11.757	11.757	2.8	ng	40439	4	11.357	287177	20.0
n-Hexadecanoic ...	11.886	4.3	ng	62339	4	11.357	287177	20.0
Trichloroacetic...	13.839	4.8	ng	90457	5	13.998	378683	20.0
Benzo[e]pyrene	15.333	3.7	ng	33568	6	15.457	181234	20.0
Octacosane	15.880	8.7	ng	78594	6	15.457	181234	20.0
unknown17.498	17.498	10.7	ng	97329	6	15.457	181234	20.0