

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
 Data File : BF130941.D
 Acq On : 02 Nov 2022 21:08
 Operator : CG\JU
 Sample : N5395-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-11-103122

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130941.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	17	25	31	rVB	480603	628808	33.44%	4.645%
2	2.340	39	43	50	rVB	38091	48991	2.60%	0.362%
3	4.034	326	331	337	rVB	209937	256999	13.67%	1.899%
4	5.151	515	521	532	rVB	422383	505803	26.89%	3.737%
5	5.540	581	587	590	rBV	1869274	1880686	100.00%	13.894%
6	5.940	651	655	660	rVB	19867	19122	1.02%	0.141%
7	6.545	752	758	761	rBV	1814440	1866363	99.24%	13.788%
8	6.922	818	822	825	rBV	537410	412819	21.95%	3.050%
9	7.316	885	889	903	rVB	130414	123212	6.55%	0.910%
10	7.487	913	918	921	rBV	1324732	1174581	62.45%	8.677%
11	7.916	987	991	1001	rBV4	12447	23539	1.25%	0.174%
12	8.110	1020	1024	1033	rBV	37382	89298	4.75%	0.660%
13	8.210	1037	1041	1043	rVV	542699	509145	27.07%	3.761%
14	8.228	1043	1044	1047	rVB	61355	36092	1.92%	0.267%
15	9.286	1219	1224	1227	rBV	1926386	1607896	85.50%	11.879%
16	9.969	1334	1340	1343	rVB	581904	481839	25.62%	3.560%
17	10.757	1470	1474	1477	rBV	1114639	899377	47.82%	6.644%
18	10.804	1479	1482	1490	rVB	29135	31836	1.69%	0.235%
19	10.880	1490	1495	1497	rBV2	20433	28079	1.49%	0.207%
20	11.457	1590	1593	1596	rBV	449254	392145	20.85%	2.897%
21	11.480	1596	1597	1601	rVB	62191	41764	2.22%	0.309%
22	11.975	1676	1681	1687	rBV3	30494	48252	2.57%	0.356%
23	12.075	1694	1698	1701	rBV4	14928	21365	1.14%	0.158%
24	12.674	1797	1800	1804	rBV	120586	98634	5.24%	0.729%
25	12.904	1834	1839	1843	rBV	89053	96169	5.11%	0.710%
26	13.045	1857	1863	1867	rBV	1089204	1039235	55.26%	7.678%
27	13.186	1884	1887	1889	rBV	32242	26072	1.39%	0.193%
28	14.027	2025	2030	2031	rBV5	30579	48706	2.59%	0.360%
29	14.110	2039	2044	2046	rBV2	395347	400796	21.31%	2.961%
30	14.133	2046	2048	2055	rVB	67782	61961	3.29%	0.458%
31	14.568	2120	2122	2125	rBV3	18380	19582	1.04%	0.145%
32	15.168	2221	2224	2227	rBV	54460	73408	3.90%	0.542%
33	15.245	2234	2237	2240	rBV2	29501	30008	1.60%	0.222%
34	15.486	2276	2278	2284	rVB	37433	44796	2.38%	0.331%
35	15.551	2286	2289	2295	rVB	47382	64649	3.44%	0.478%
36	15.621	2296	2301	2305	rBV	318114	403955	21.48%	2.984%

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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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

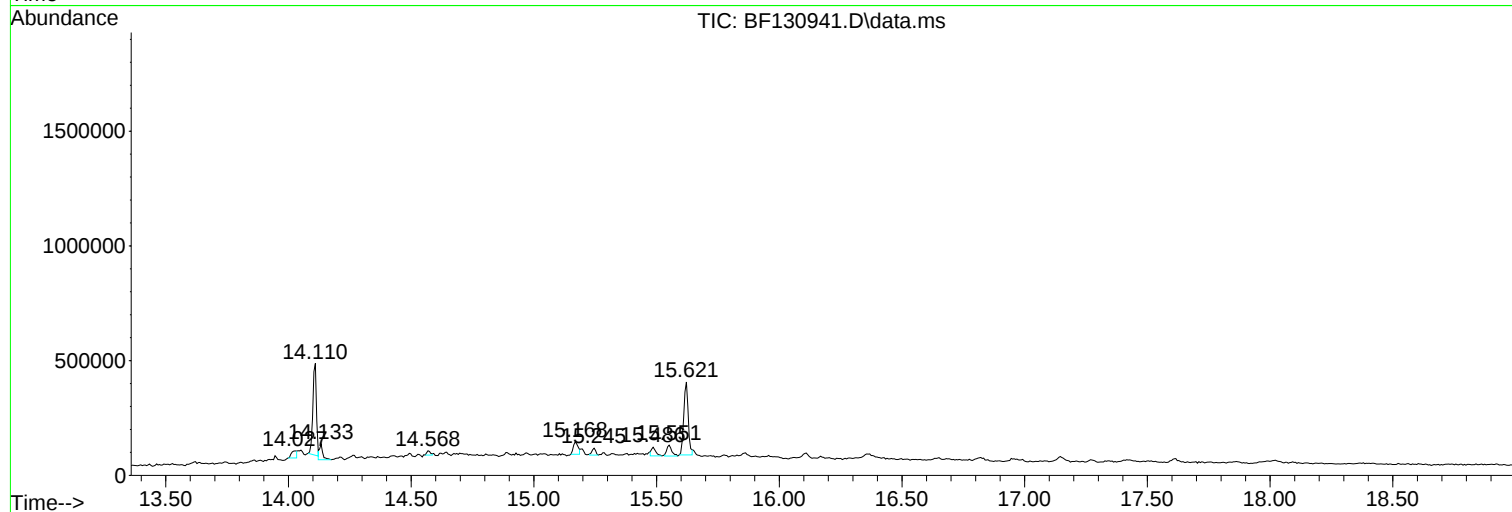
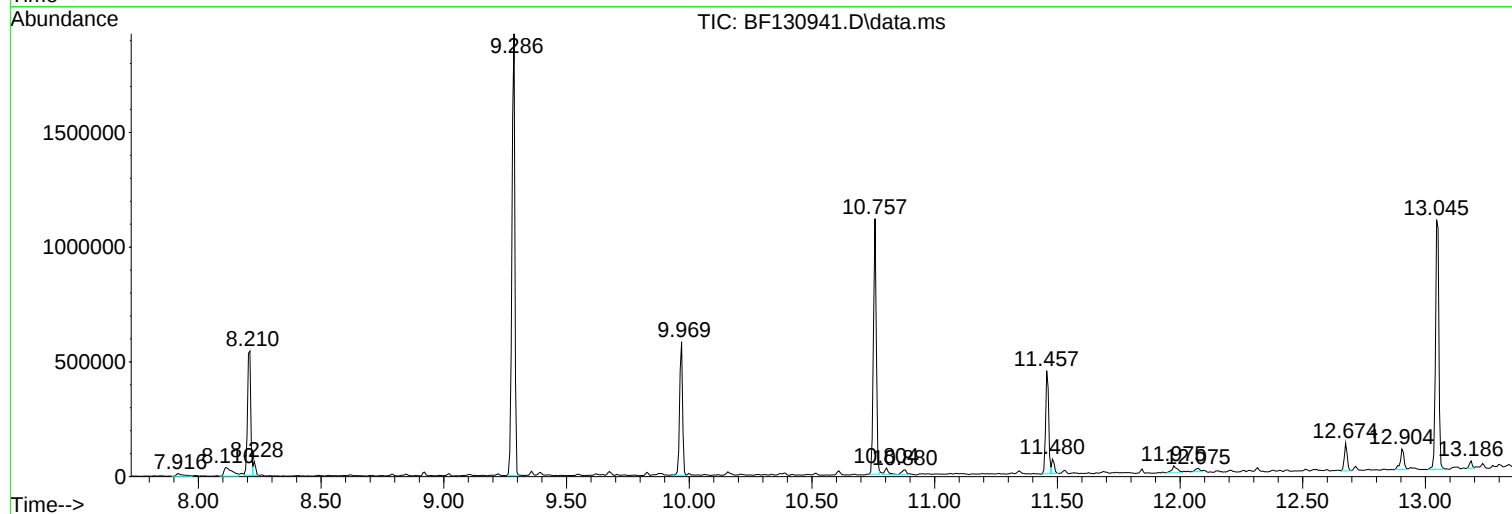
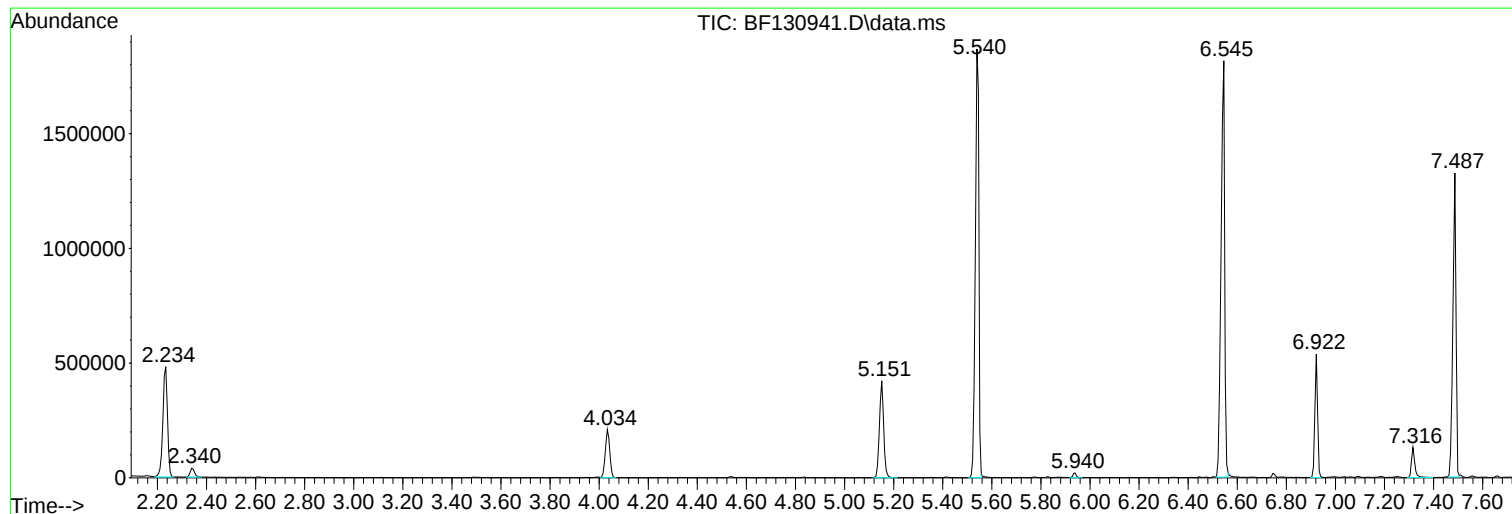
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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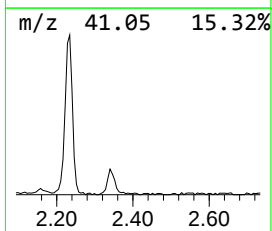
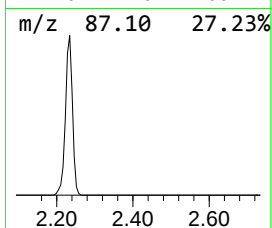
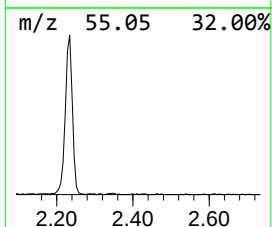
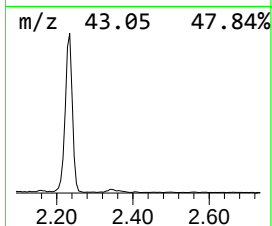
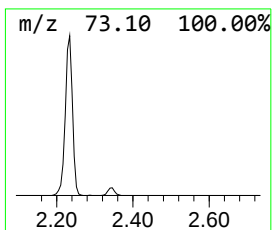
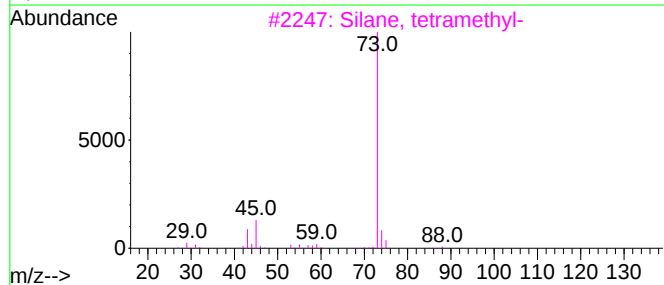
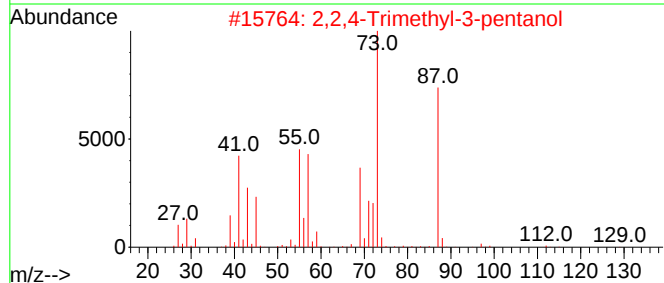
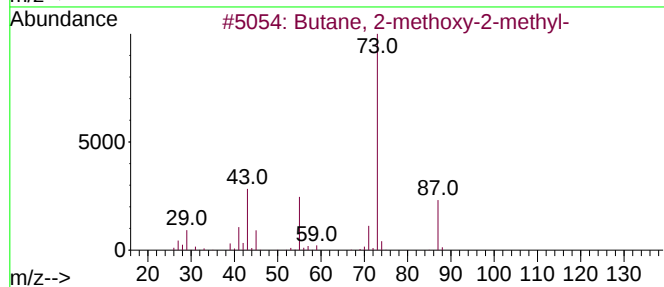
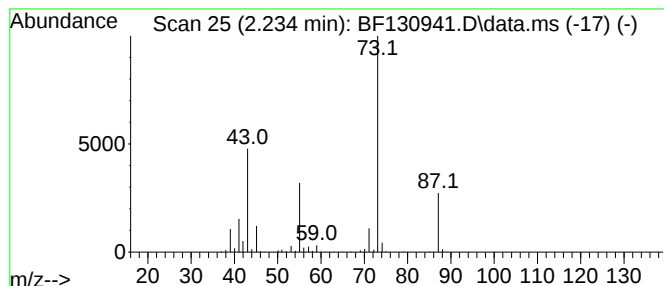
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.234	30.46 ng	628808	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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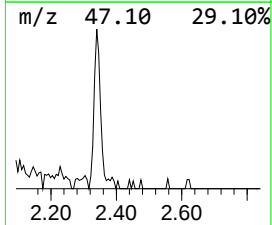
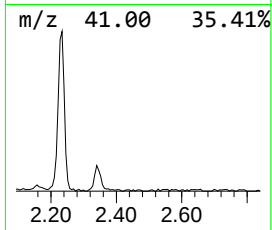
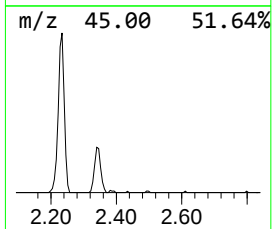
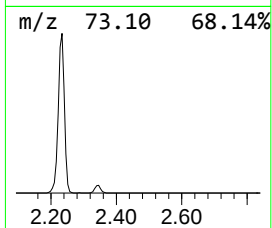
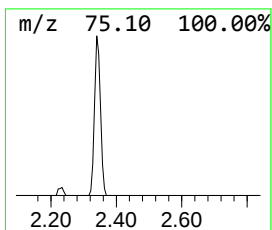
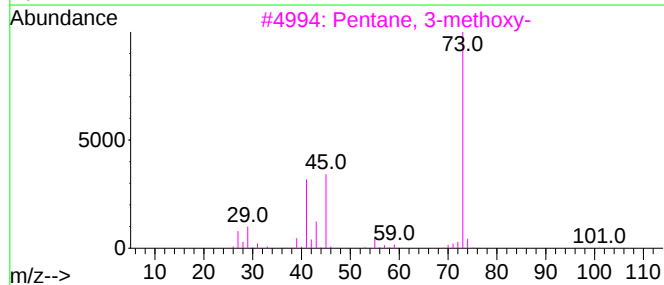
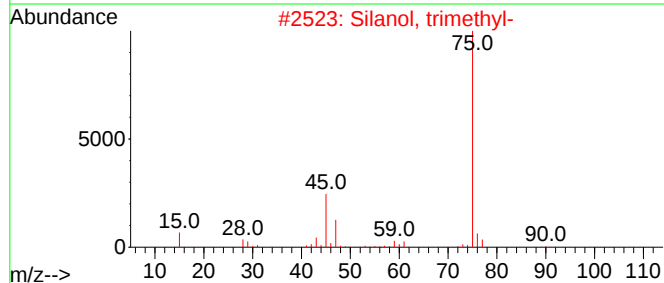
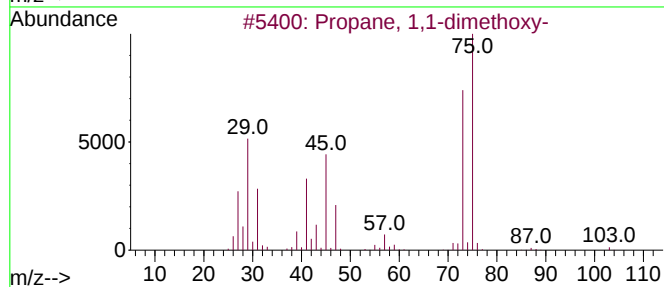
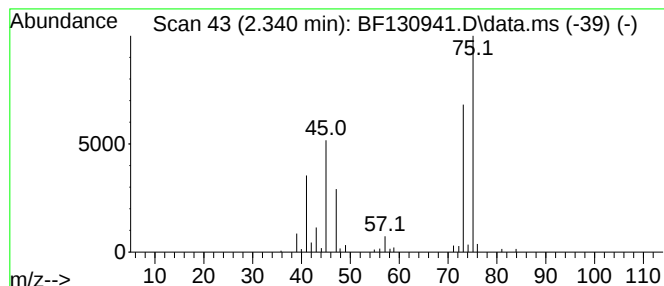
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.340	2.37 ng	48991	1,4-Dichlorobenzene-d4	6.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4		Hydrazine, propyl-	74	C3H10N2	005039-61-2	9
5		Methane, trimethoxy-	106	C4H10O3	000149-73-5	9



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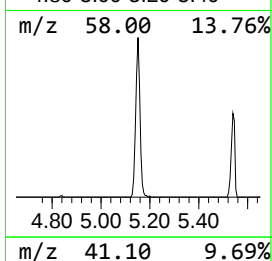
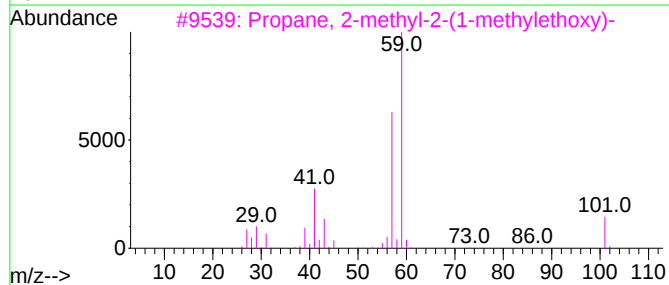
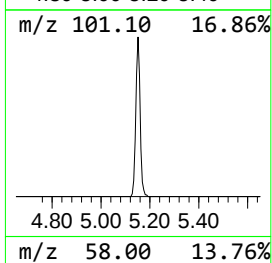
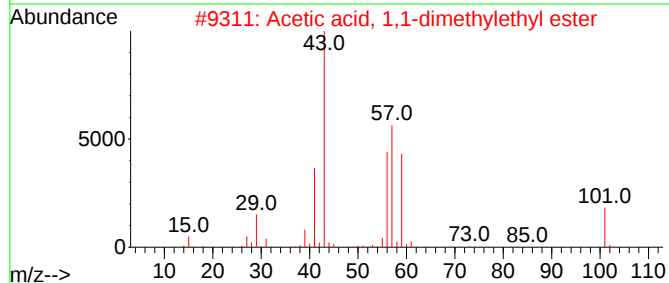
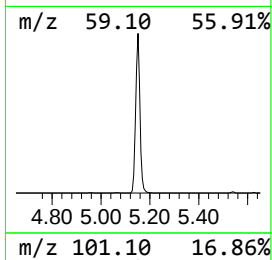
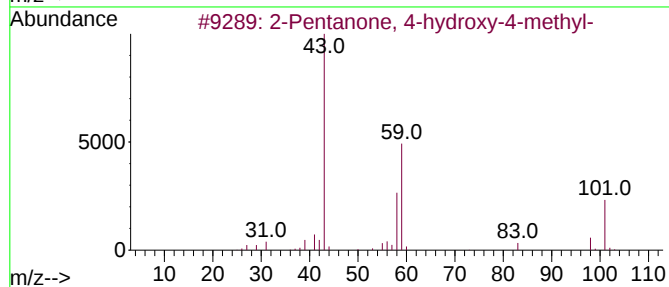
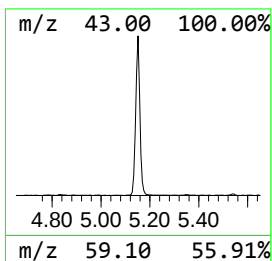
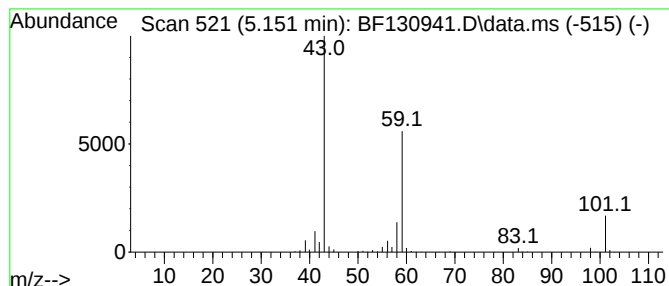
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	24.50 ng	505803	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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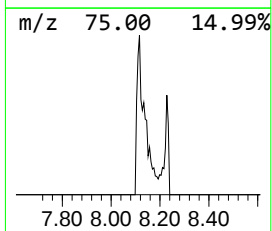
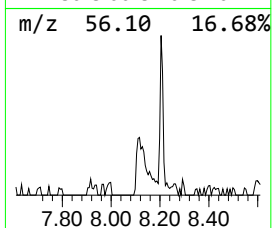
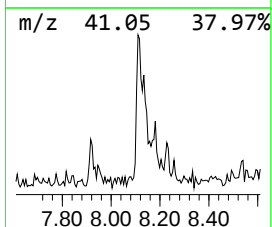
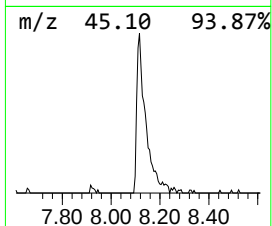
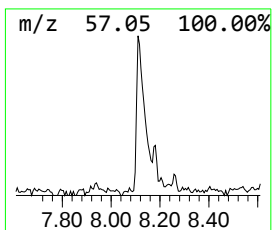
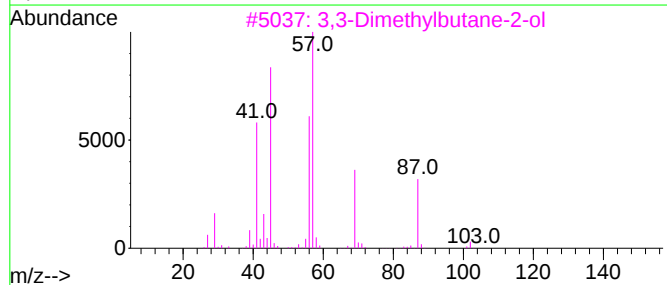
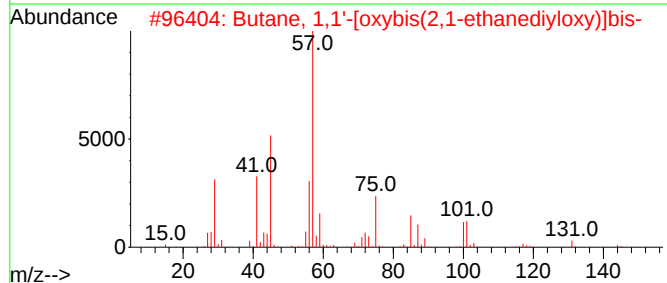
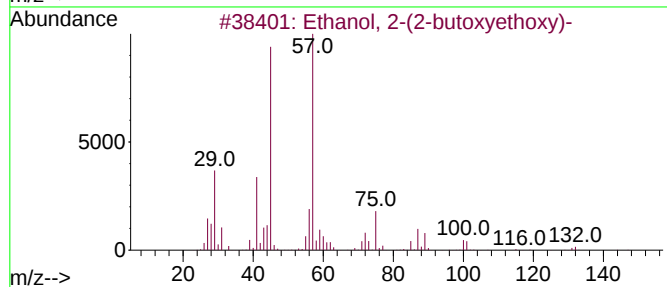
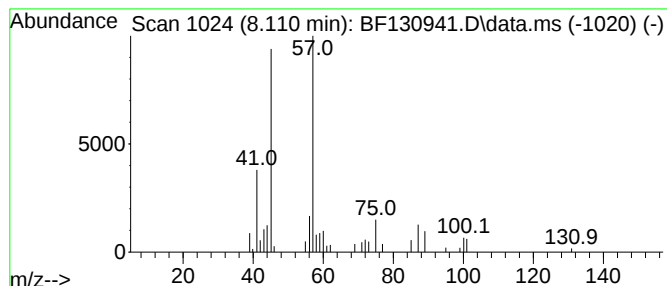
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	3.51 ng	89298	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47



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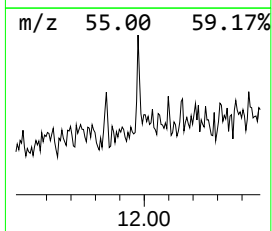
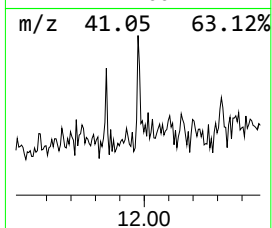
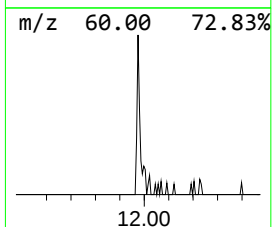
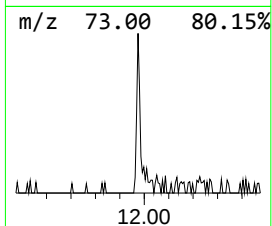
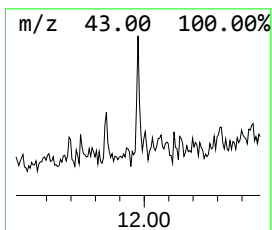
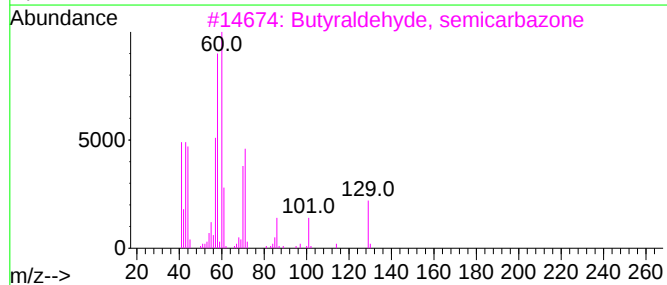
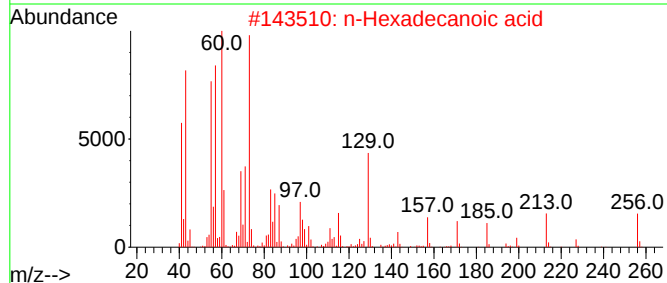
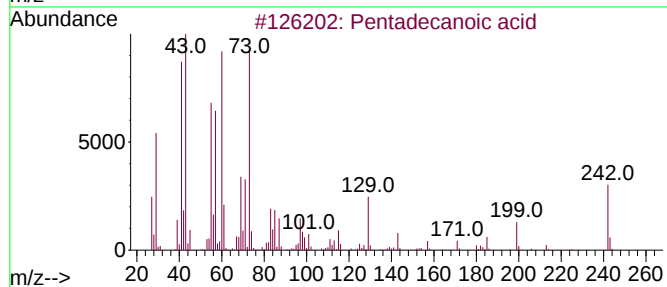
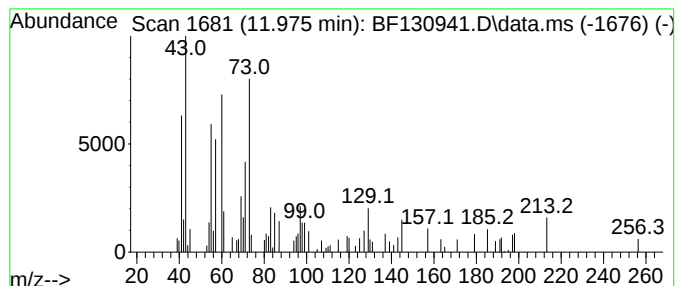
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	2.46 ng	48252	Phenanthrene-d10	11.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
3			Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	46
4			n-Decanoic acid	172	C10H20O2	000334-48-5	43
5			Dodecanoic acid	200	C12H24O2	000143-07-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130941.D
Acq On : 02 Nov 2022 21:08
Operator : CG\JU
Sample : N5395-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

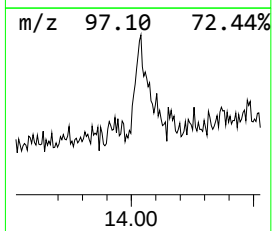
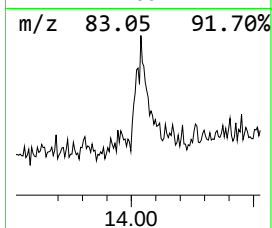
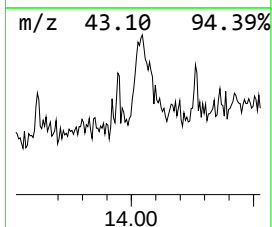
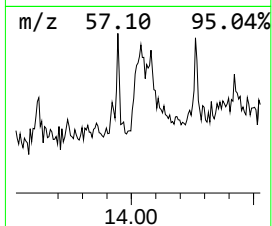
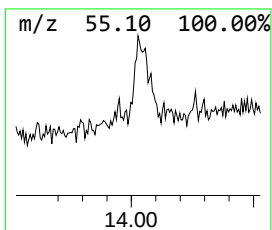
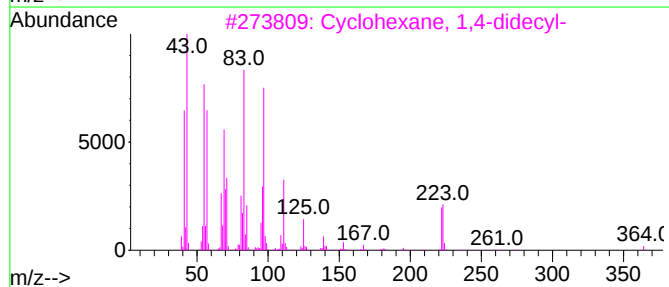
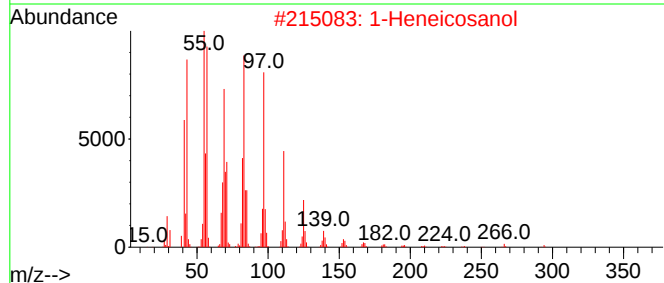
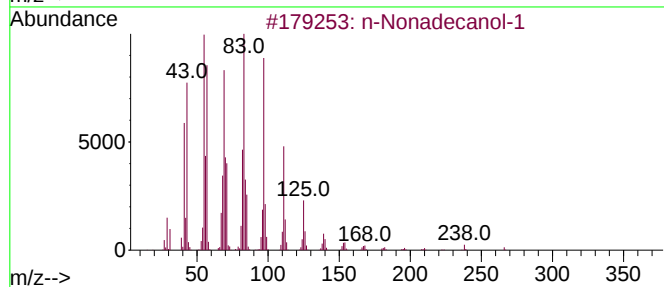
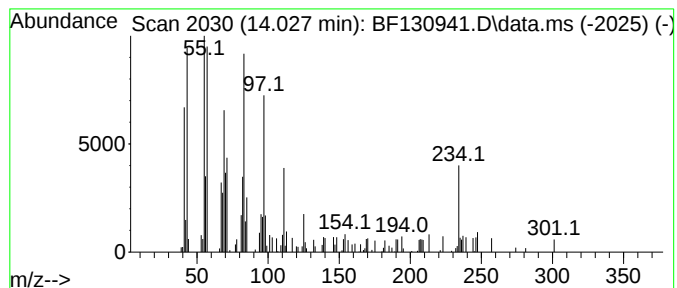
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BNA_F
ClientSampleId :
S-11-103122

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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-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.027	2.43 ng	48706	Chrysene-d12	14.110	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	89
2	1-Heneicosanol	312	C21H44O	015594-90-8	89
3	Cyclohexane, 1,4-didecyl-	364	C26H52	055334-20-8	76
4	1-Heptacosanol	396	C27H56O	002004-39-9	68
5	Behenic alcohol	326	C22H46O	000661-19-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130941.D
Acq On : 02 Nov 2022 21:08
Operator : CG\JU
Sample : N5395-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-11-103122

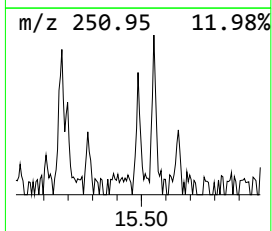
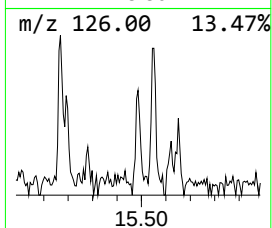
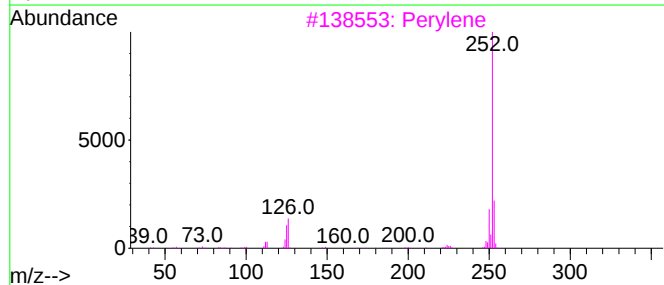
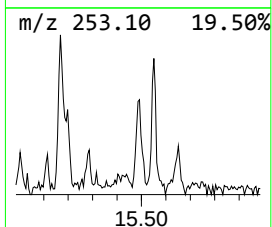
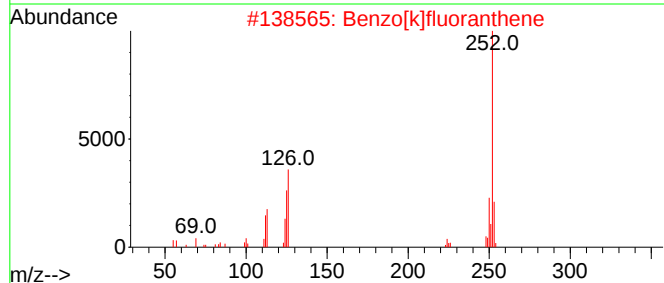
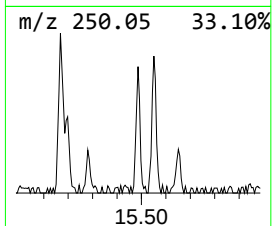
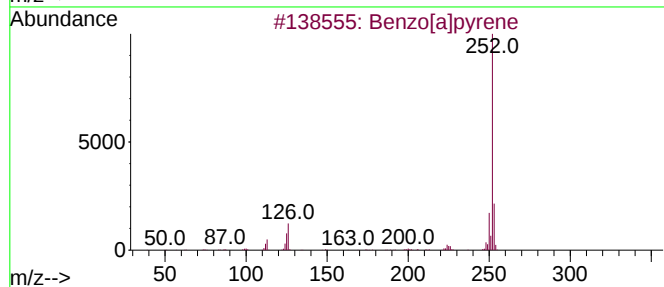
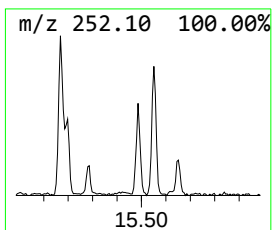
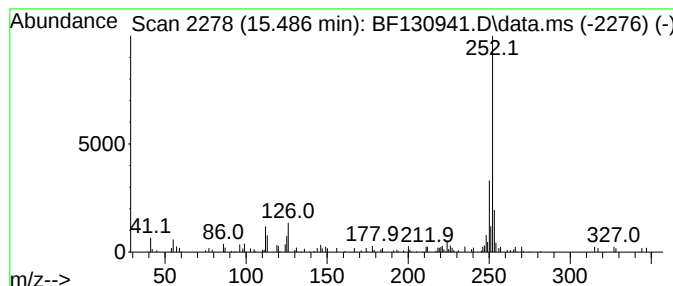
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	2.22 ng	44796	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	81
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
3			Perylene	252	C20H12	000198-55-0	72
4			Benzo[e]pyrene	252	C20H12	000192-97-2	72
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130941.D
Acq On : 02 Nov 2022 21:08
Operator : CG\JU
Sample : N5395-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-11-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.234	30.5	ng	628808	1	6.922	412819	20.0
Propane, 1,1-di...	2.340	2.4	ng	48991	1	6.922	412819	20.0
2-Pentanone, 4-...	5.151	24.5	ng	505803	1	6.922	412819	20.0
Ethanol, 2-(2-b...	8.110	3.5	ng	89298	2	8.210	509145	20.0
Pentadecanoic acid	11.975	2.5	ng	48252	4	11.457	392145	20.0
n-Nonadecanol-1	14.027	2.4	ng	48706	5	14.110	400796	20.0
Perylene	15.486	2.2	ng	44796	6	15.621	403955	20.0