

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
 Data File : BF140111.D
 Acq On : 29 Oct 2024 14:42
 Operator : RC/JU
 Sample : P4578-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WB-305-BOT-1

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	9	17	24	rVB	1266994	2007518	74.34%	8.638%
2	3.999	318	324	336	rVB	21469	35342	1.31%	0.152%
3	5.116	510	514	523	rVB	17523	27735	1.03%	0.119%
4	5.504	574	580	586	rBV	1779539	2384772	88.31%	10.261%
5	6.504	744	750	768	rVB	1747782	2501850	92.64%	10.765%
6	6.887	810	815	820	rBV	618303	750575	27.79%	3.229%
7	7.445	902	910	919	rBV	1177559	1572985	58.25%	6.768%
8	7.698	947	953	960	rVB2	75341	114812	4.25%	0.494%
9	7.904	980	988	992	rBV2	21628	34582	1.28%	0.149%
10	8.169	1025	1033	1040	rBV	783185	1032254	38.22%	4.441%
11	8.381	1063	1069	1076	rBV	28092	40961	1.52%	0.176%
12	8.757	1128	1133	1137	rVB	47651	57250	2.12%	0.246%
13	9.239	1210	1215	1224	rBV	1998750	2700474	100.00%	11.619%
14	9.322	1224	1229	1234	rVB	67396	90403	3.35%	0.389%
15	9.639	1279	1283	1290	rVB3	26856	49288	1.83%	0.212%
16	9.851	1312	1319	1323	rBV	44304	59039	2.19%	0.254%
17	9.922	1326	1331	1343	rVB	887799	1144822	42.39%	4.926%
18	10.351	1396	1404	1408	rBV2	20249	30758	1.14%	0.132%
19	10.633	1447	1452	1459	rBV	488870	640623	23.72%	2.756%
20	10.710	1459	1465	1479	rVV	1375616	1827006	67.66%	7.861%
21	10.945	1501	1505	1512	rVB	37178	47221	1.75%	0.203%
22	11.410	1579	1584	1592	rBV	898380	1137268	42.11%	4.893%
23	11.475	1592	1595	1600	rVB2	37803	49234	1.82%	0.212%
24	11.639	1617	1623	1631	rBV8	14214	41207	1.53%	0.177%
25	11.933	1666	1673	1685	rBV	275405	452288	16.75%	1.946%
26	12.022	1685	1688	1697	rVB2	17953	40666	1.51%	0.175%
27	12.186	1712	1716	1724	rVB3	63064	81770	3.03%	0.352%
28	12.433	1754	1758	1765	rBV3	16929	32600	1.21%	0.140%
29	12.663	1794	1797	1802	rVB	27428	35969	1.33%	0.155%
30	12.722	1802	1807	1813	rBV2	28864	48440	1.79%	0.208%
31	12.857	1826	1830	1834	rBV2	16240	34169	1.27%	0.147%
32	12.998	1848	1854	1859	rBV	1895286	2439680	90.34%	10.497%
33	13.227	1889	1893	1900	rBV2	19363	27811	1.03%	0.120%
34	13.569	1947	1951	1960	rBV	25218	39911	1.48%	0.172%
35	13.898	2002	2007	2026	rBV	78496	201410	7.46%	0.867%
36	14.057	2028	2034	2046	rVB	481682	648129	24.00%	2.789%

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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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.221	2058	2062	2067	rBV	22027	28968	1.07%	0.125%
38	14.539	2112	2116	2121	rBV	19358	27398	1.01%	0.118%
39	15.557	2282	2289	2302	rBV	451534	724396	26.82%	3.117%

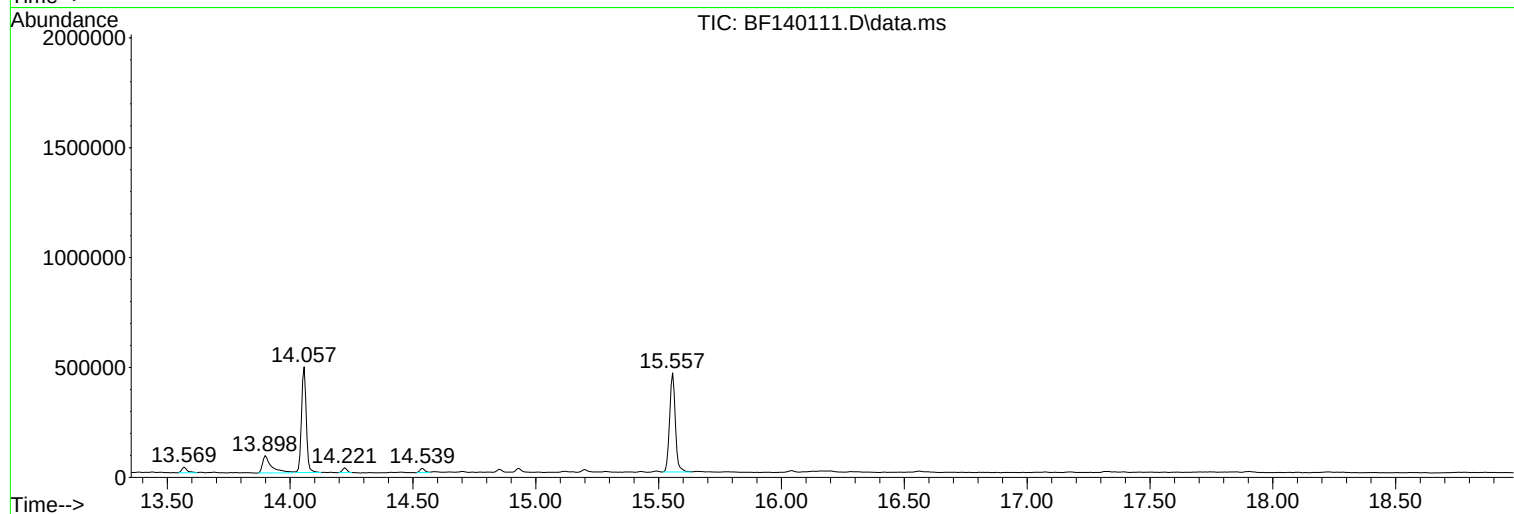
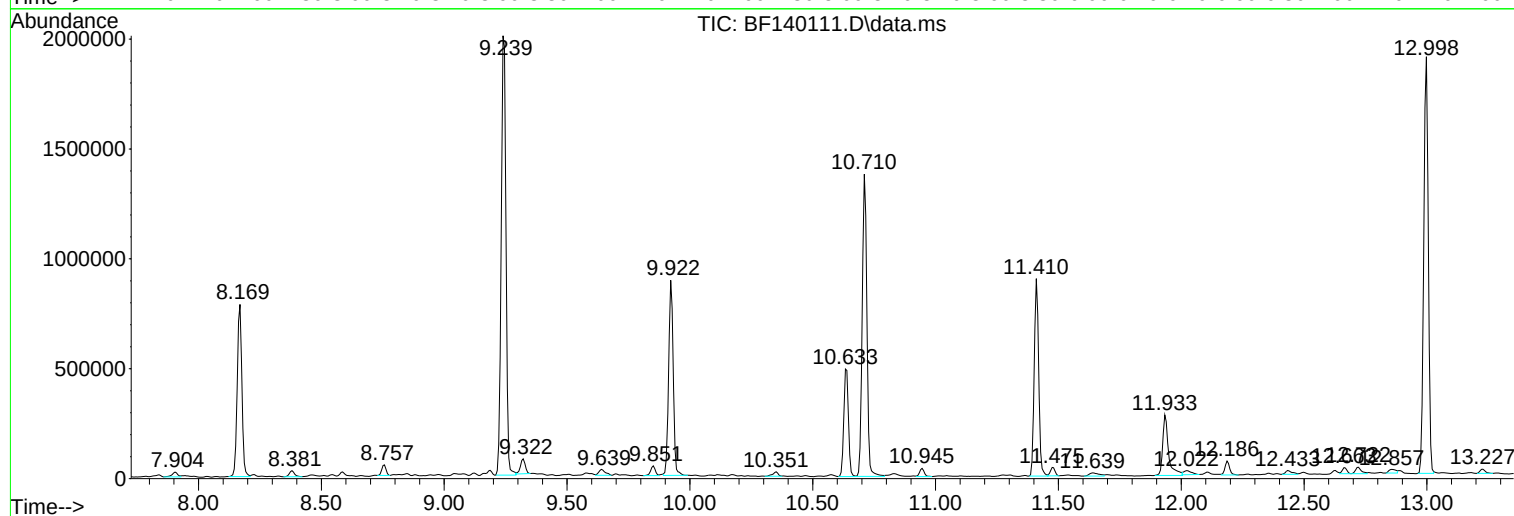
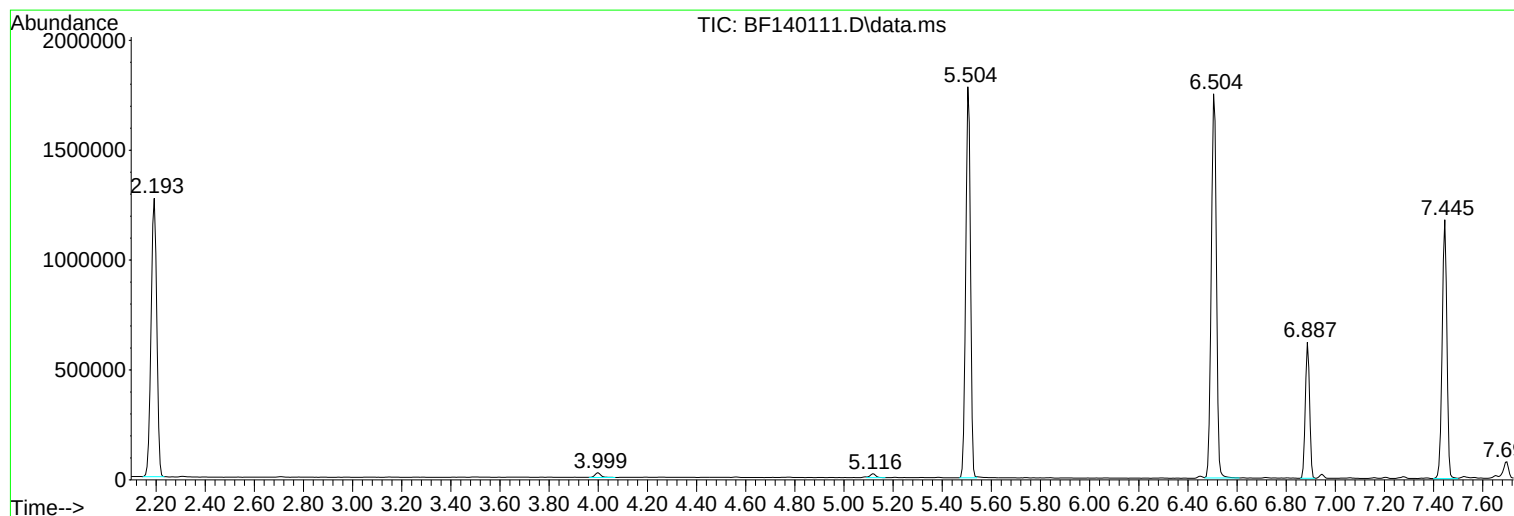
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
BNA_F
ClientSampleId :
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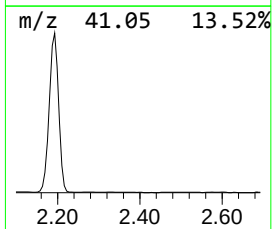
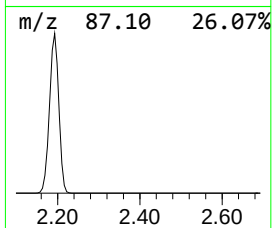
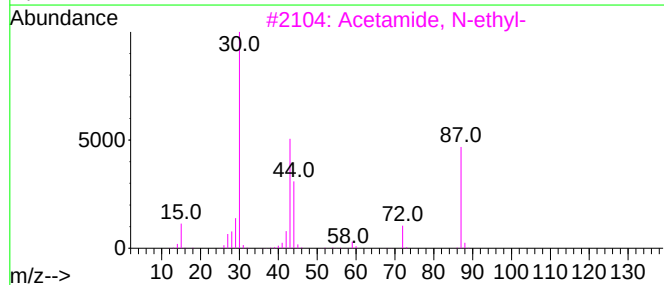
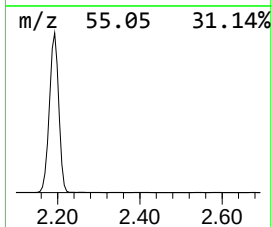
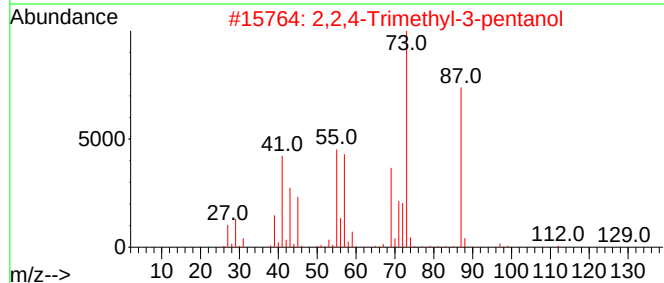
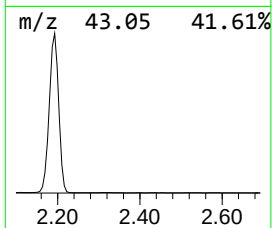
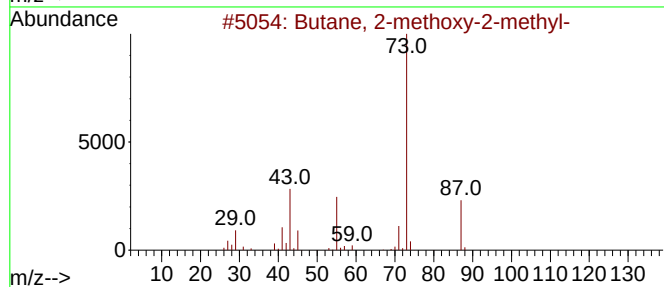
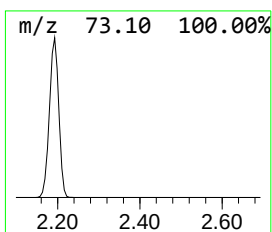
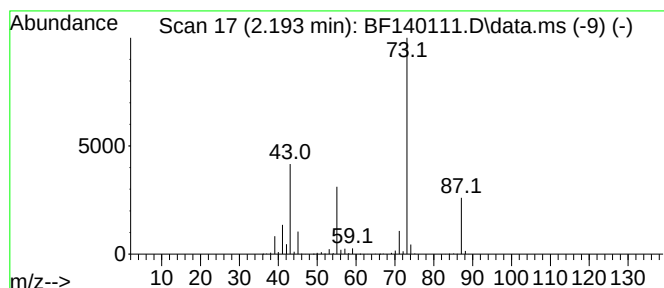
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	53.49 ng	2007520	1,4-Dichlorobenzene-d4	6.887

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	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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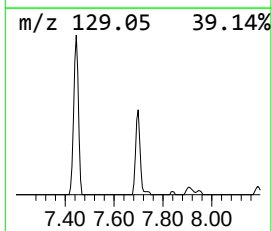
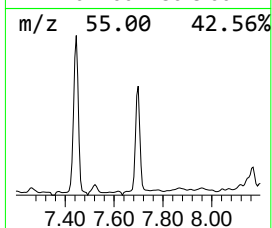
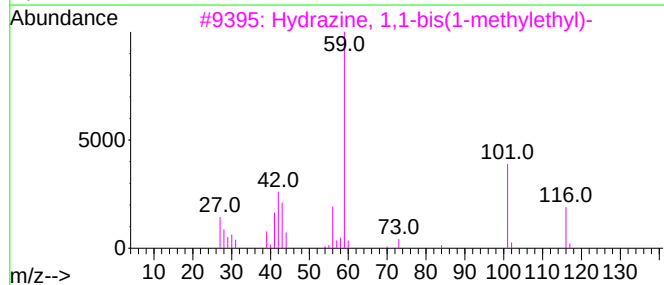
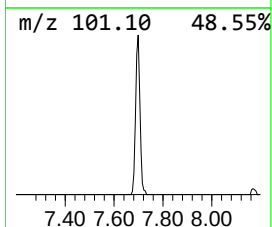
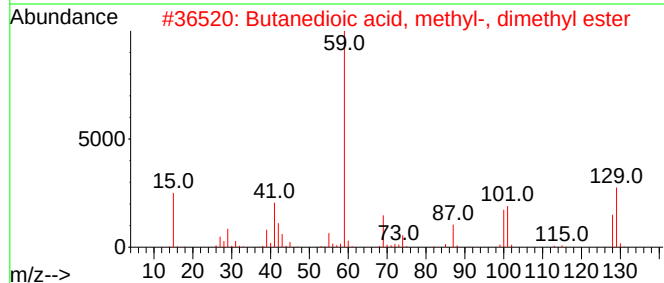
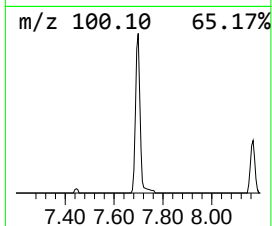
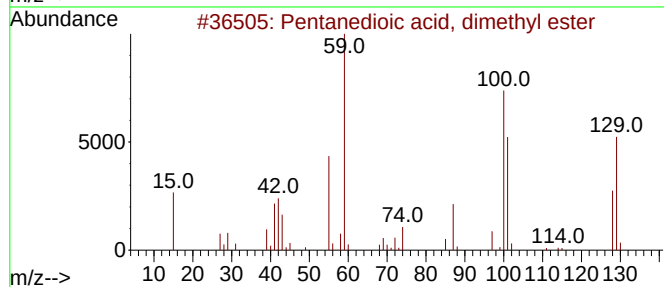
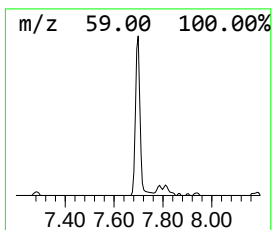
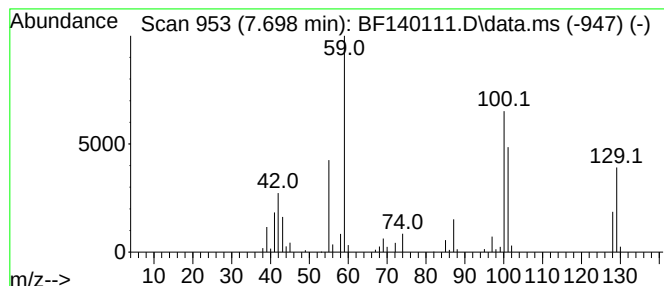
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Peak Number 2 Pentanedioic acid, dimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.22 ng	114812	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	42
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
4			Hydrazine, (1-methylethyl)-	74	C3H10N2	002257-52-5	27
5			Hydrazine, trimethyl-	74	C3H10N2	001741-01-1	27



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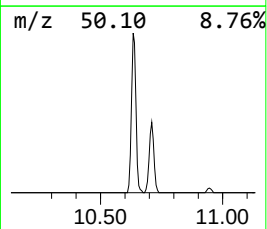
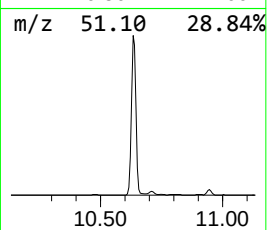
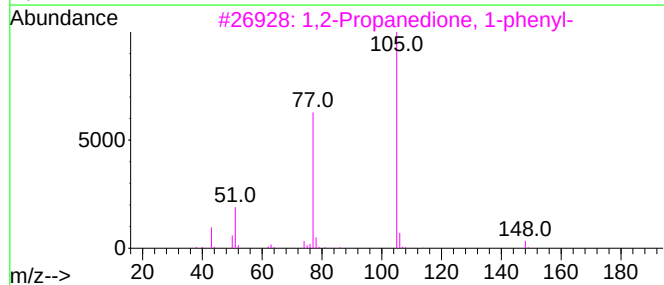
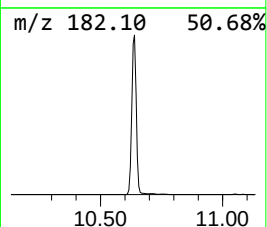
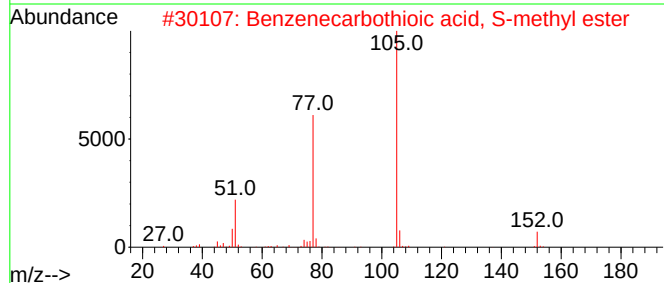
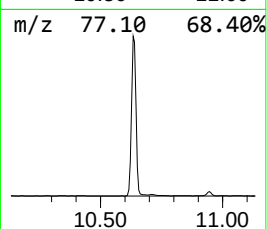
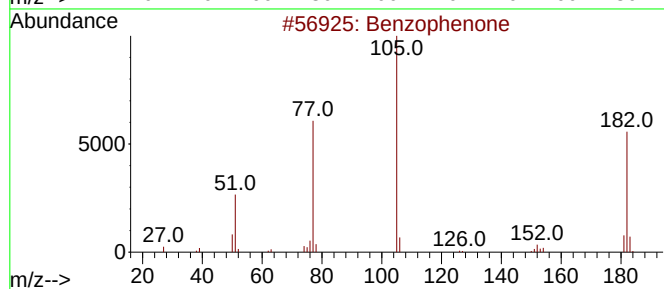
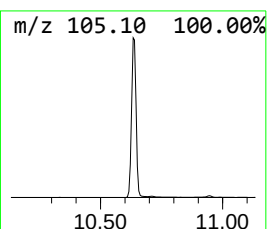
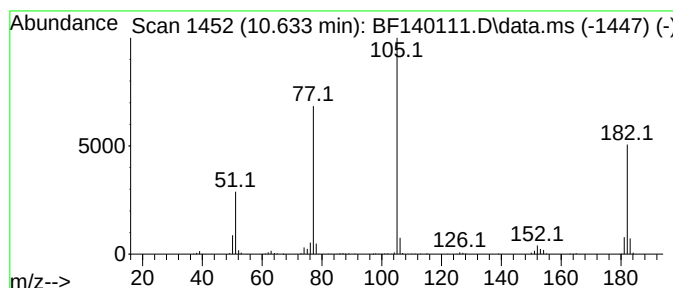
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.633	11.19 ng	640623	Acenaphthene-d10	9.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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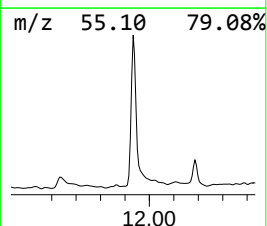
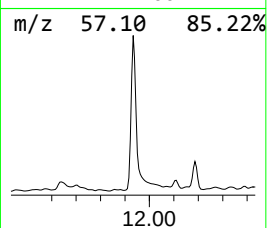
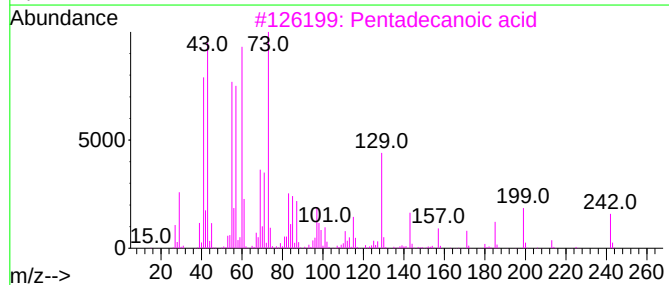
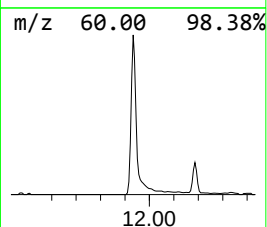
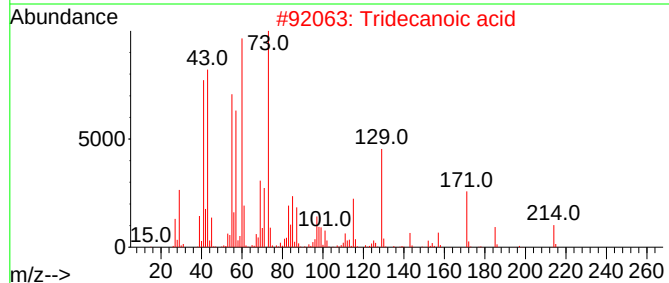
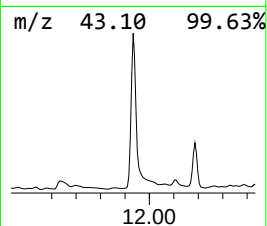
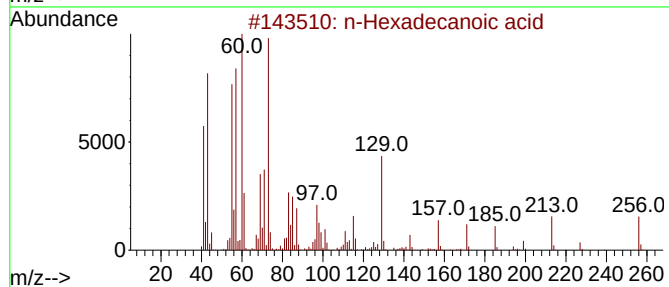
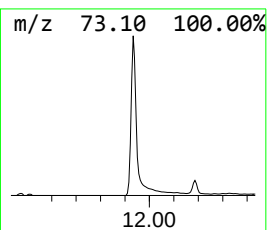
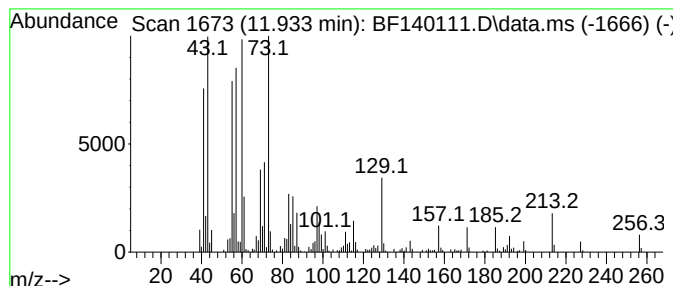
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	7.95 ng	452288	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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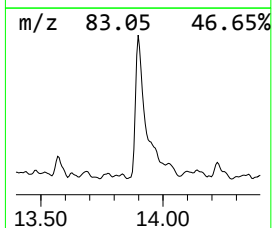
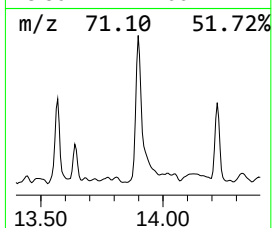
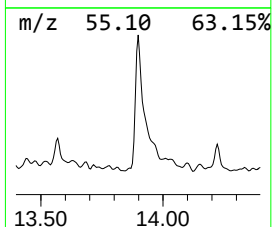
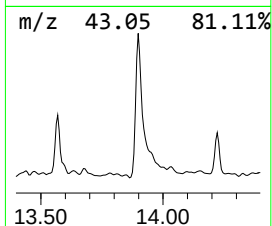
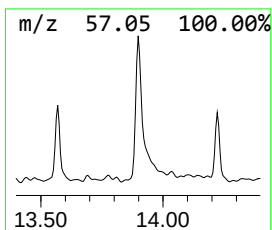
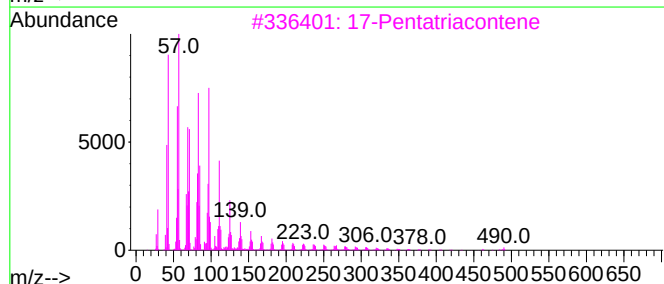
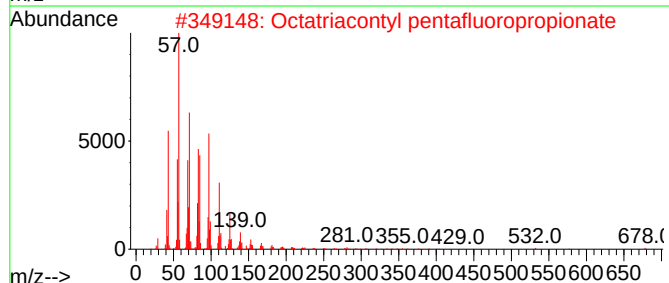
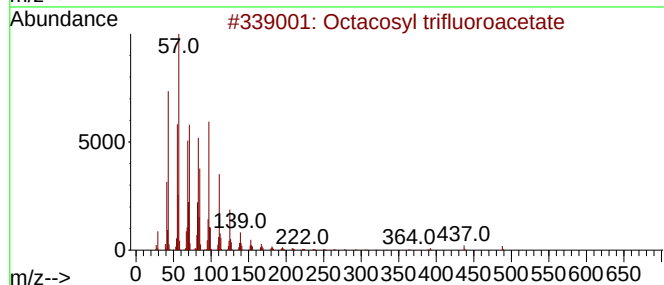
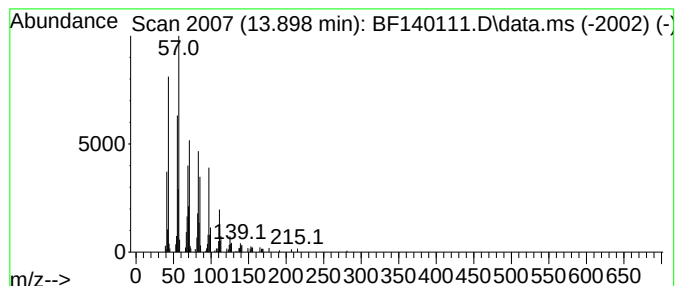
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	6.22 ng	201410	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91
3			17-Pentatriacontene	491	C35H70	006971-40-0	91
4			Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	91
5			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140111.D
Acq On : 29 Oct 2024 14:42
Operator : RC/JU
Sample : P4578-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-BOT-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.193	53.5	ng	2007520	1	6.887	750575	20.0
Pentanedioic ac...	7.698	2.2	ng	114812	2	8.169	1032250	20.0
Benzophenone	10.633	11.2	ng	640623	3	9.922	1144820	20.0
n-Hexadecanoic ...	11.933	8.0	ng	452288	4	11.410	1137270	20.0
Octacosyl trifl...	13.898	6.2	ng	201410	5	14.057	648129	20.0