

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
 Data File : BF140168.D
 Acq On : 30 Oct 2024 19:58
 Operator : RC/JU
 Sample : P4594-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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: BF140168.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	14	22	rVB	805971	1271455	76.15%	9.311%
2	5.504	574	580	585	rBV	1247911	1669725	100.00%	12.227%
3	6.504	744	750	766	rVB	1219296	1629119	97.57%	11.930%
4	6.887	809	815	820	rVB	406489	519841	31.13%	3.807%
5	7.439	903	909	914	rBV	803122	1025928	61.44%	7.513%
6	7.692	948	952	960	rVB	37284	45213	2.71%	0.331%
7	8.163	1025	1032	1037	rBV	501525	620282	37.15%	4.542%
8	8.375	1062	1068	1076	rBV2	13692	18497	1.11%	0.135%
9	9.239	1209	1215	1220	rBV	1194836	1477653	88.50%	10.821%
10	9.322	1224	1229	1234	rBV	25799	33135	1.98%	0.243%
11	9.639	1279	1283	1291	rBV4	11206	22532	1.35%	0.165%
12	9.851	1312	1319	1324	rBV	33586	45443	2.72%	0.333%
13	9.922	1324	1331	1337	rVB	456732	579476	34.70%	4.243%
14	10.357	1398	1405	1409	rBV	31685	45320	2.71%	0.332%
15	10.575	1436	1442	1448	rBV	12297	21283	1.27%	0.156%
16	10.639	1448	1453	1460	rBV	65372	86149	5.16%	0.631%
17	10.716	1460	1466	1471	rBV	607091	810171	48.52%	5.933%
18	10.833	1480	1486	1495	rBV	32702	54858	3.29%	0.402%
19	11.280	1556	1562	1565	rBV	23819	33045	1.98%	0.242%
20	11.416	1580	1585	1592	rBV	442527	555795	33.29%	4.070%
21	11.480	1593	1596	1601	rVB2	12941	17567	1.05%	0.129%
22	11.710	1631	1635	1639	rBV	18159	21438	1.28%	0.157%
23	11.945	1668	1675	1684	rBV	126506	209202	12.53%	1.532%
24	12.121	1701	1705	1708	rBV3	17506	23740	1.42%	0.174%
25	12.510	1767	1771	1777	rVB2	13537	18731	1.12%	0.137%
26	12.674	1796	1799	1805	rVB3	20507	26067	1.56%	0.191%
27	12.733	1805	1809	1815	rBV	35802	62609	3.75%	0.458%
28	12.827	1821	1825	1830	rVB	57761	75336	4.51%	0.552%
29	12.886	1831	1835	1837	rBV2	15259	21420	1.28%	0.157%
30	13.010	1850	1856	1865	rBV	1132713	1443230	86.44%	10.569%
31	13.539	1943	1946	1950	rBV	43027	55782	3.34%	0.408%
32	13.921	2007	2011	2023	rBV	65486	136618	8.18%	1.000%
33	14.080	2033	2038	2044	rVB	446223	588236	35.23%	4.308%
34	15.604	2292	2297	2302	rBV	259219	391040	23.42%	2.864%

Sum of corrected areas: 13655936

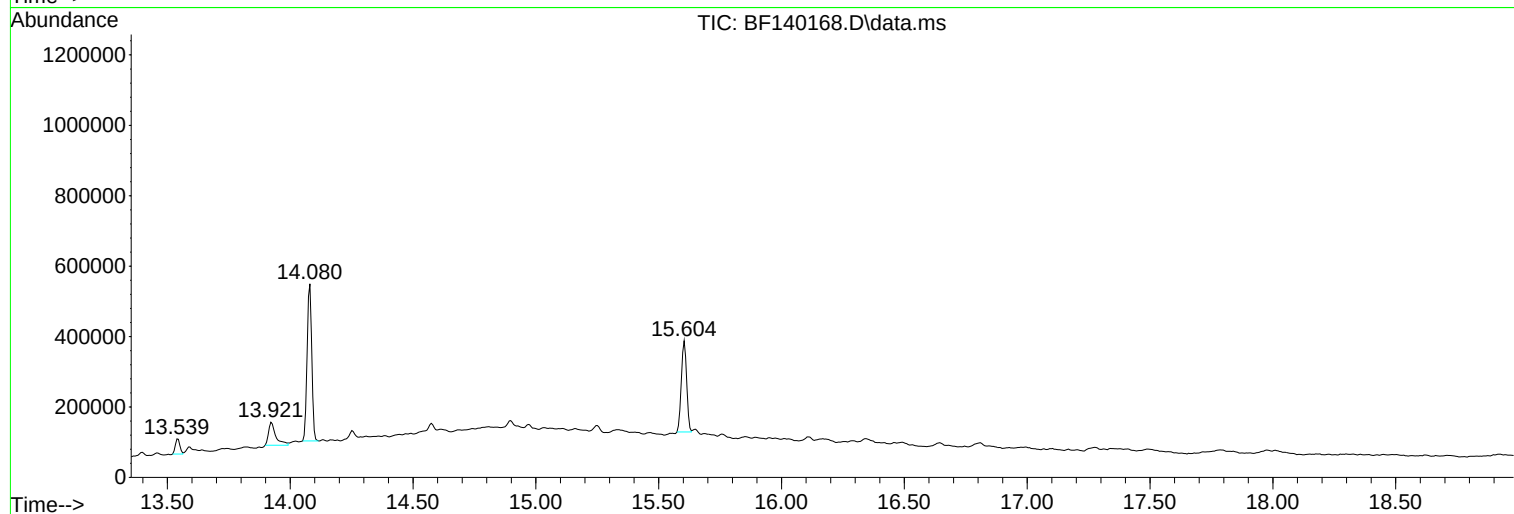
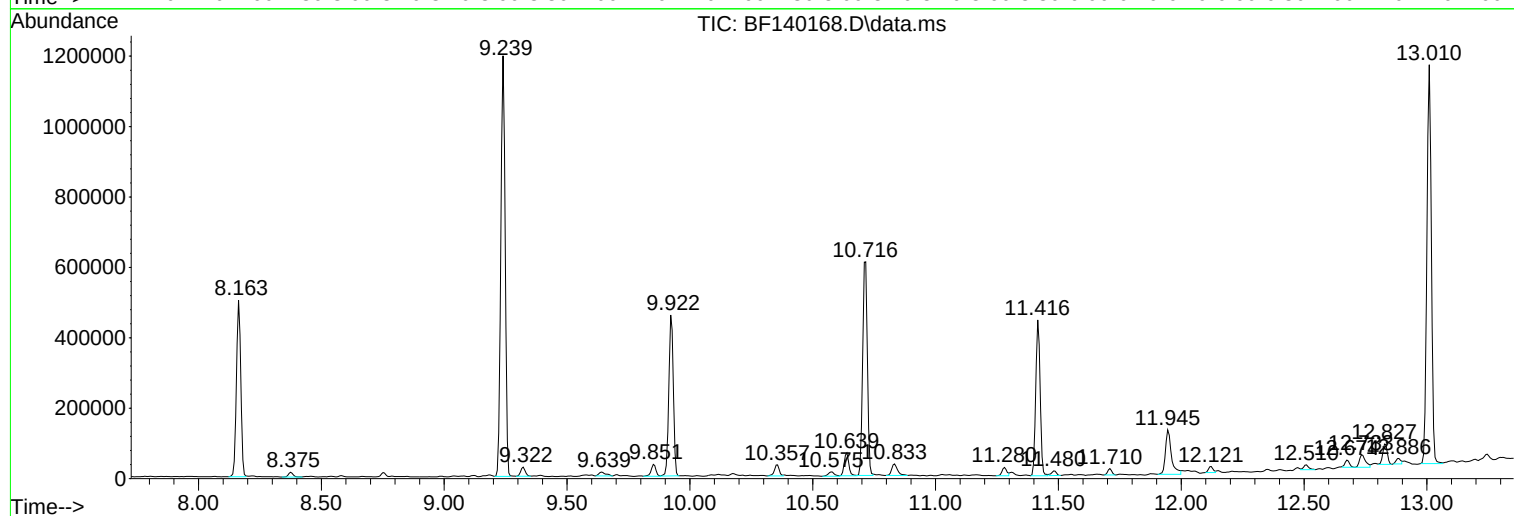
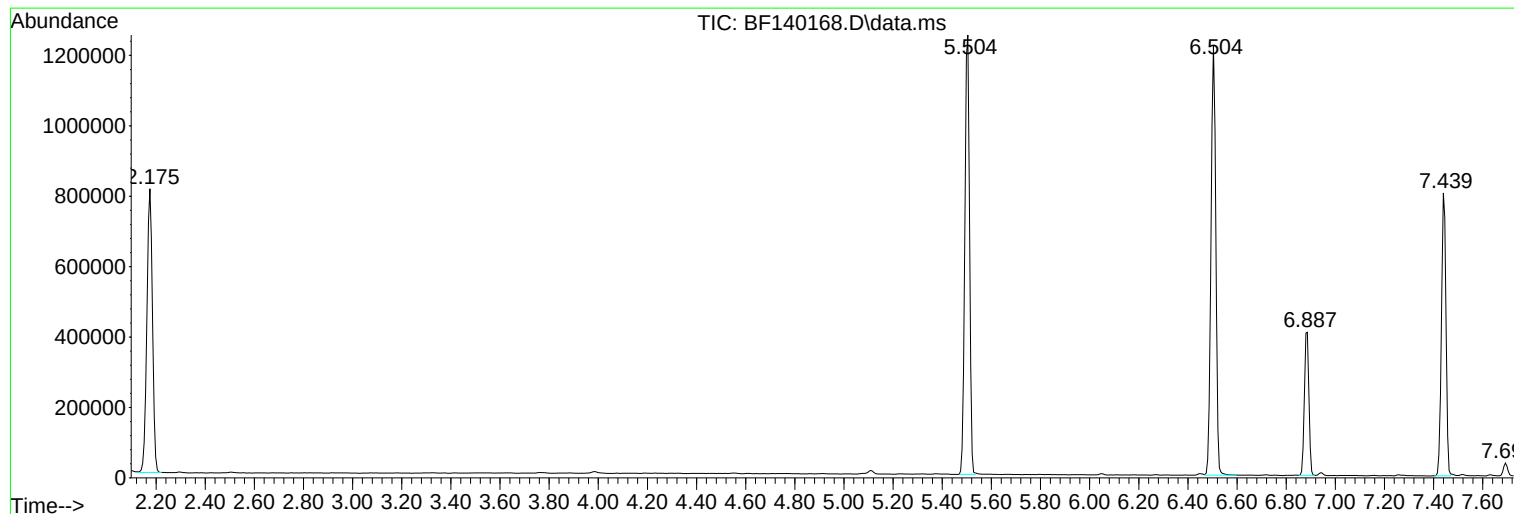
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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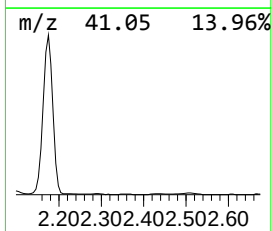
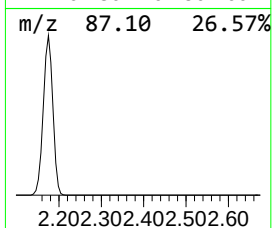
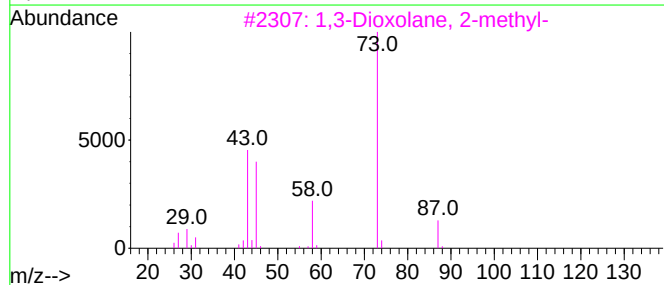
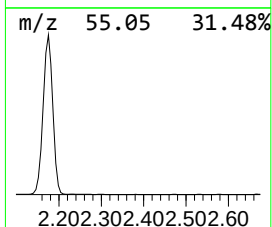
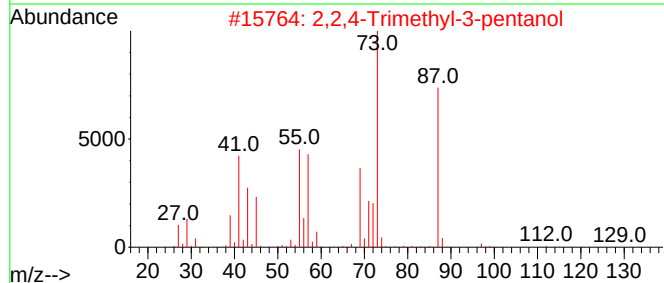
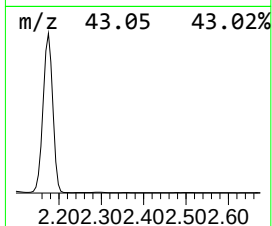
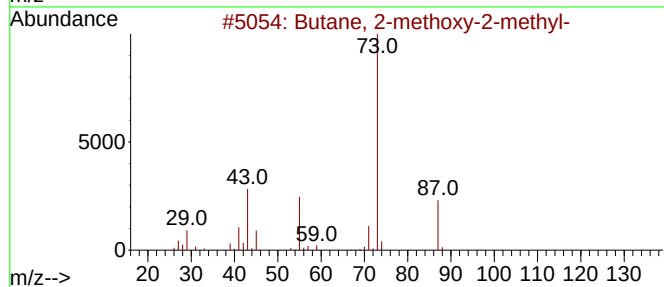
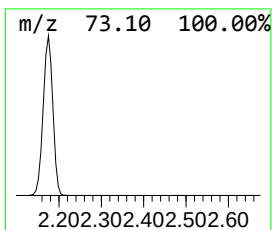
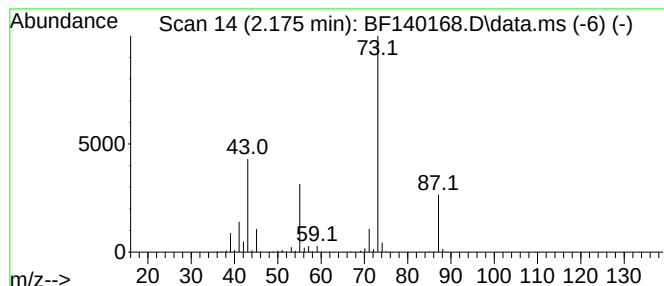
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	48.92 ng	1271460	1,4-Dichlorobenzene-d4	6.886

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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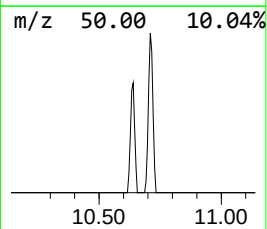
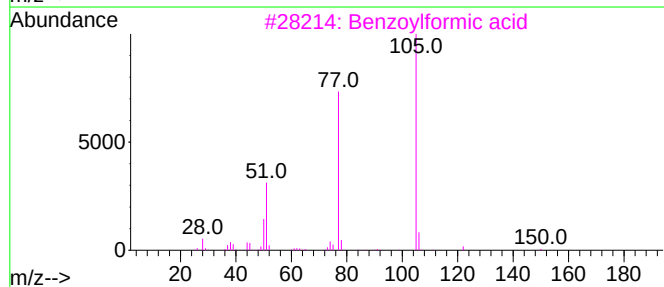
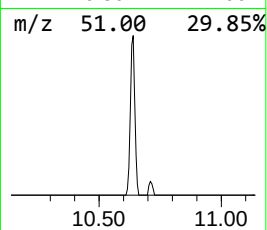
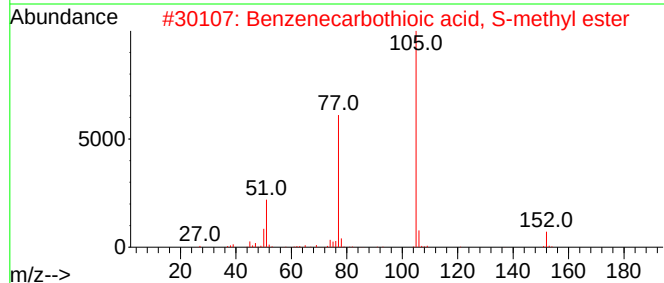
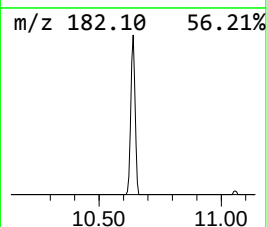
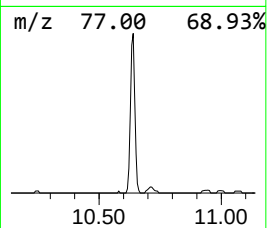
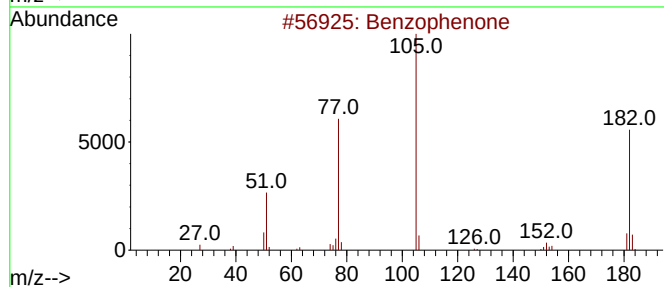
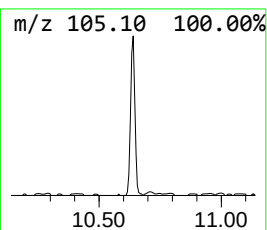
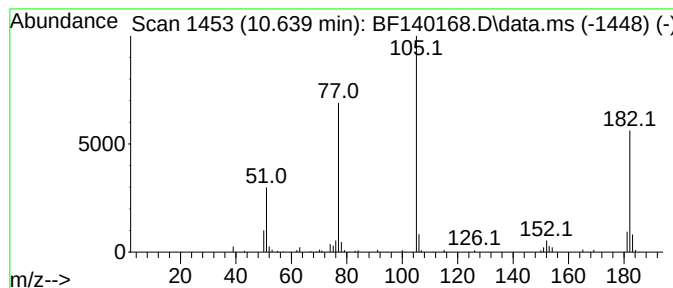
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	2.97 ng	86149	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			Benzoylformic acid	150	C8H6O3	000611-73-4	49
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			Benzoic acid, 2-(benzoylthio)thi...	341	C17H11NO3S2	1000258-72-7	47



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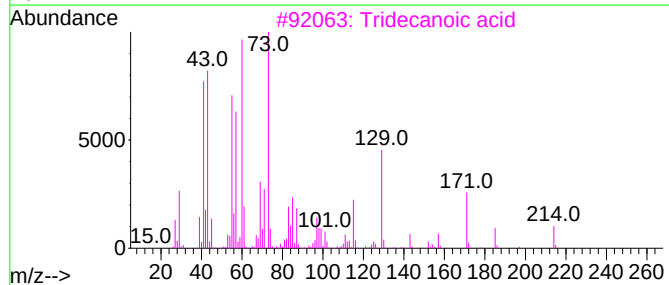
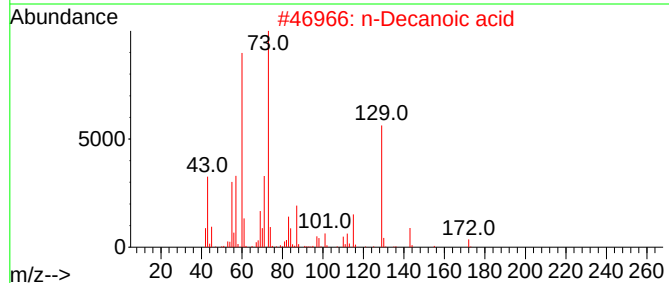
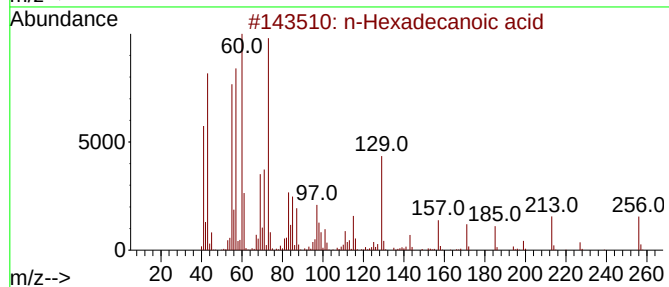
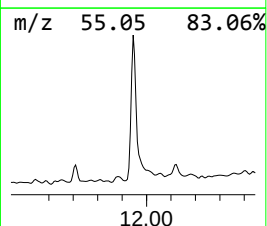
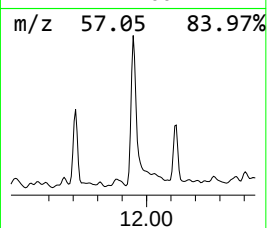
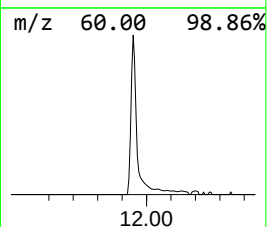
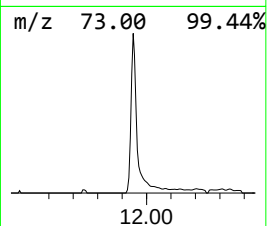
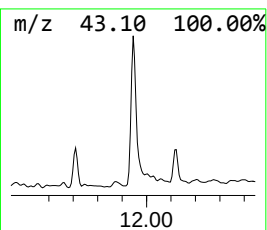
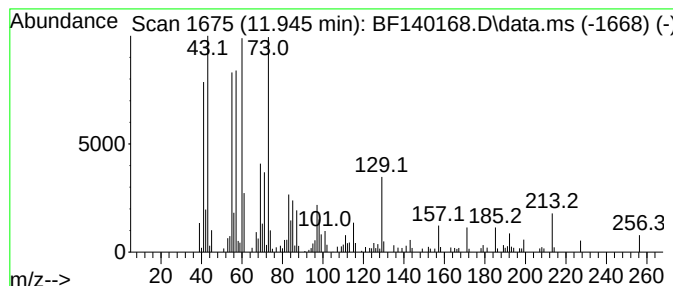
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	7.53 ng	209202	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	92
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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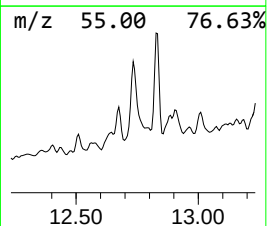
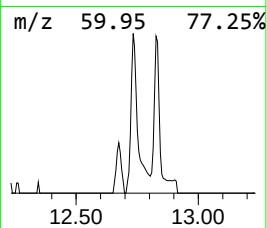
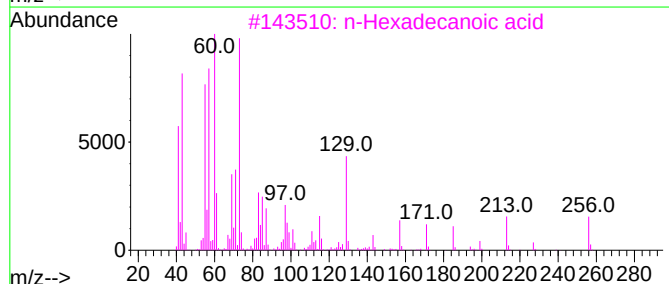
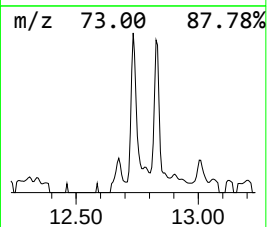
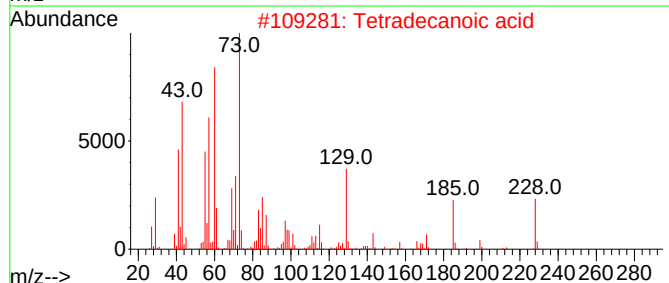
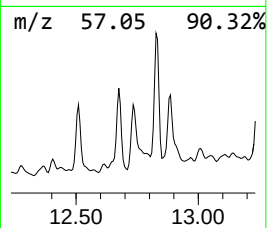
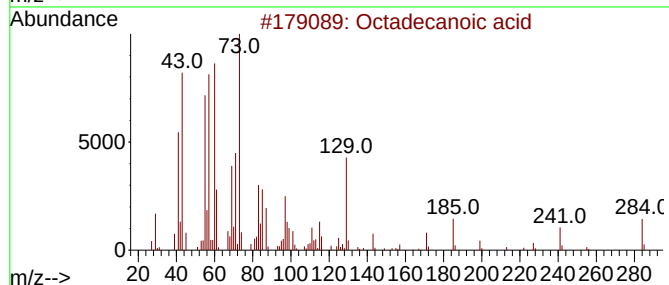
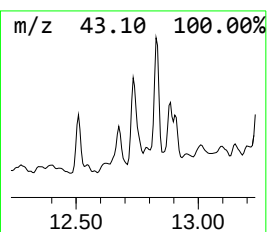
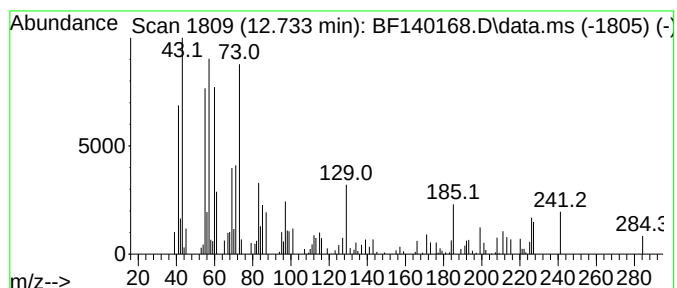
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.25 ng	62609	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	86
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58



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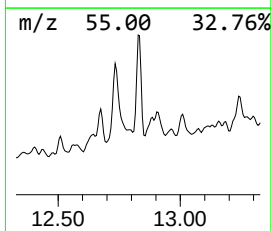
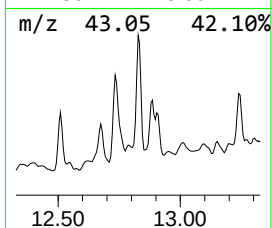
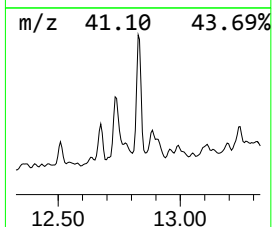
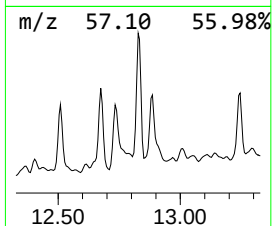
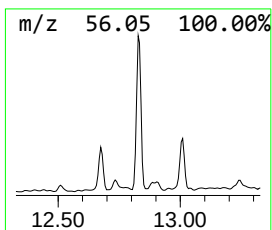
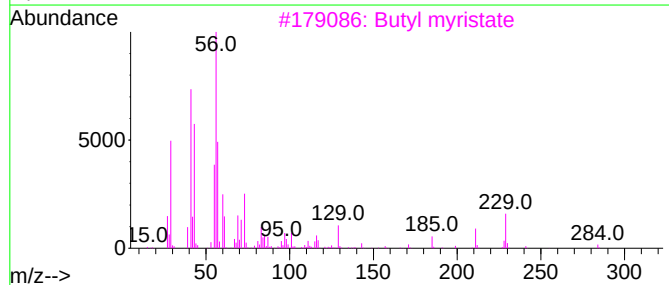
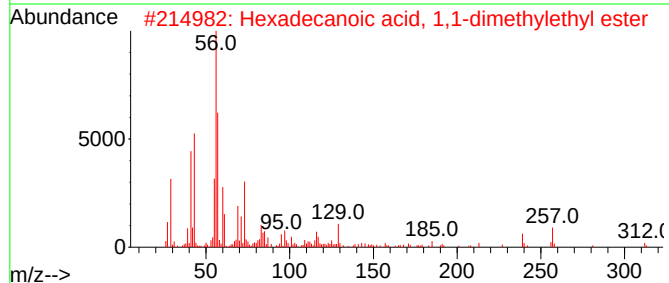
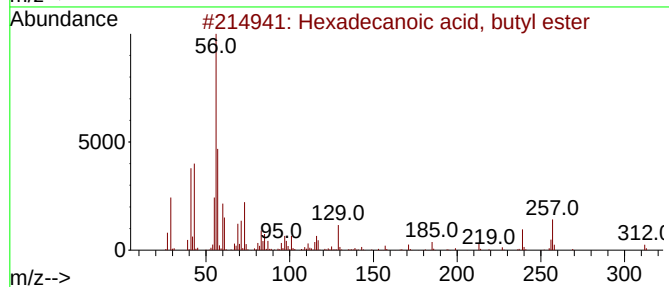
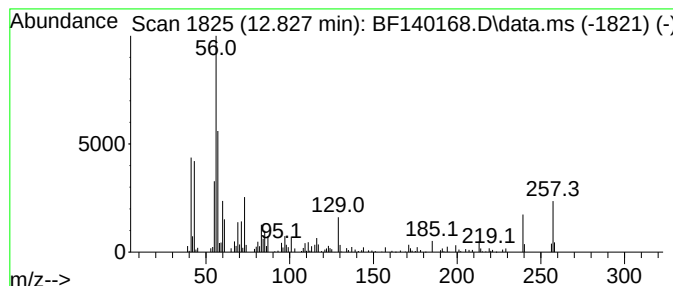
Instrument :
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.827	2.56 ng	75336	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Butyl myristate	284	C18H36O2	000110-36-1	68
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	53
5	Isobutyl laurate	256	C16H32O2	037811-72-6	49



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TP-4

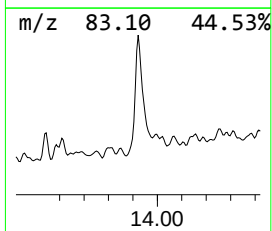
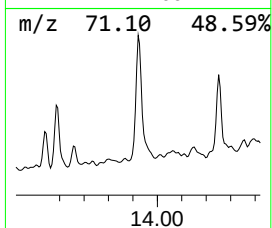
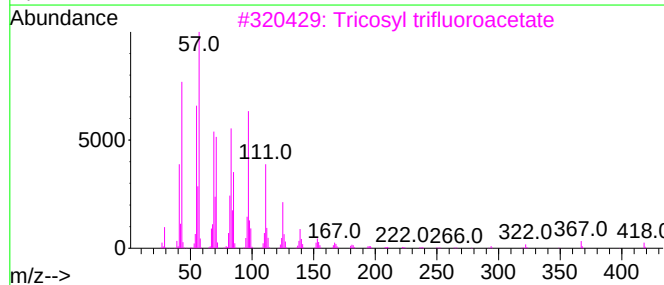
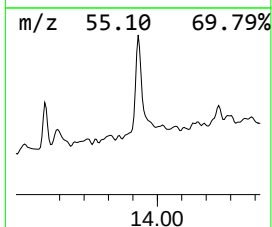
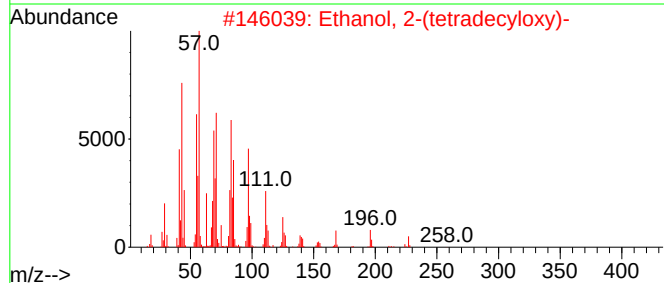
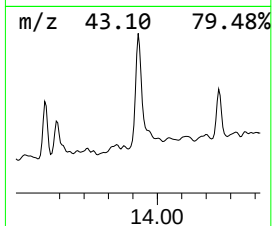
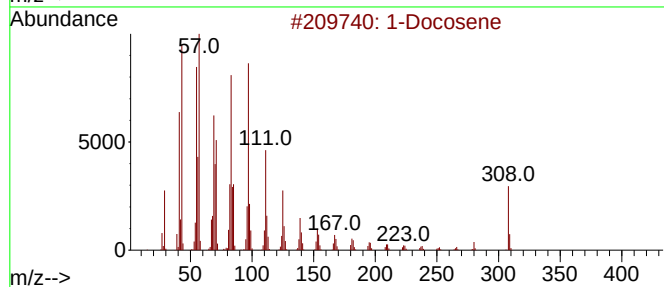
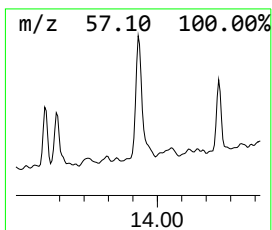
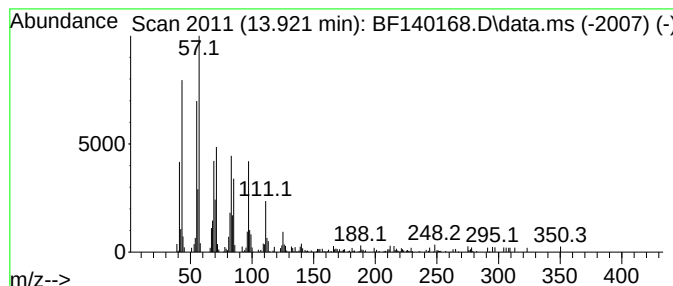
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	4.65 ng	136618	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	Ethanol, 2-(tetradecyloxy)-			258	C16H34O2	002136-70-1	91
3	Tricosyl trifluoroacetate			436	C25H47F3O2	1000351-75-1	91
4	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	91
5	Heptafluorobutyric acid, n-octad...			466	C22H37F7O2	000400-57-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140168.D
Acq On : 30 Oct 2024 19:58
Operator : RC/JU
Sample : P4594-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.175	48.9	ng	1271460	1	6.886	519841	20.0
Benzophenone	10.639	3.0	ng	86149	3	9.922	579476	20.0
n-Hexadecanoic ...	11.945	7.5	ng	209202	4	11.416	555795	20.0
Octadecanoic acid	12.733	2.3	ng	62609	4	11.416	555795	20.0
Hexadecanoic ac...	12.827	2.6	ng	75336	5	14.080	588236	20.0
1-Docosene	13.921	4.7	ng	136618	5	14.080	588236	20.0