

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
 Data File : BF139296.D
 Acq On : 10 Sep 2024 13:30
 Operator : RC/JU
 Sample : P3905-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-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-BF090424.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	11	18	25	rVB	1471344	2346305	64.75%	8.309%
2	2.540	59	76	83	rVB	22648	61513	1.70%	0.218%
3	5.110	504	513	523	rBV	153879	253315	6.99%	0.897%
4	5.510	574	581	586	rBV	2145873	2979181	82.21%	10.550%
5	6.516	744	752	757	rBV	2149068	3191324	88.07%	11.302%
6	6.887	810	815	820	rBV	609426	730012	20.15%	2.585%
7	7.451	904	911	916	rBV	1501033	2040598	56.31%	7.226%
8	7.698	949	953	959	rVB	68804	83056	2.29%	0.294%
9	8.169	1027	1033	1038	rBV	768353	943582	26.04%	3.342%
10	8.386	1063	1070	1074	rBV	29109	37680	1.04%	0.133%
11	9.245	1210	1216	1221	rBV	2851065	3623700	100.00%	12.833%
12	9.922	1326	1331	1336	rBV	832199	1038286	28.65%	3.677%
13	10.639	1447	1453	1460	rBV	280343	346678	9.57%	1.228%
14	10.710	1460	1465	1482	rBV	1621410	2160607	59.62%	7.651%
15	11.410	1579	1584	1592	rBV2	815098	1130363	31.19%	4.003%
16	11.933	1664	1673	1684	rBV	335235	552598	15.25%	1.957%
17	12.021	1684	1688	1697	rVB3	45667	92451	2.55%	0.327%
18	12.621	1785	1790	1795	rBV	278112	348799	9.63%	1.235%
19	12.721	1803	1807	1814	rBV	60114	93890	2.59%	0.332%
20	12.851	1822	1829	1835	rBV	249714	349281	9.64%	1.237%
21	12.998	1845	1854	1859	rBV	2085560	2652569	73.20%	9.394%
22	13.068	1861	1866	1874	rVB3	22785	40894	1.13%	0.145%
23	13.174	1877	1884	1888	rVB	31024	63726	1.76%	0.226%
24	13.245	1889	1896	1899	rBV2	21134	39144	1.08%	0.139%
25	13.898	2002	2007	2018	rBV3	96992	201022	5.55%	0.712%
26	14.045	2026	2032	2044	rVB2	495776	887133	24.48%	3.142%
27	14.433	2090	2098	2101	rBV	38384	76468	2.11%	0.271%
28	14.557	2117	2119	2127	rVB3	23483	49915	1.38%	0.177%
29	14.815	2158	2163	2169	rBV2	68606	117970	3.26%	0.418%
30	14.910	2175	2179	2186	rBV4	16906	39235	1.08%	0.139%
31	15.092	2204	2210	2220	rBV	165376	381992	10.54%	1.353%
32	15.198	2225	2228	2233	rVB	28924	40734	1.12%	0.144%
33	15.398	2257	2262	2267	rVB	92116	138269	3.82%	0.490%
34	15.457	2267	2272	2278	rBV	125456	192585	5.31%	0.682%
35	15.527	2278	2284	2297	rVB	386216	665451	18.36%	2.357%
36	16.998	2528	2534	2543	rVB2	58131	129472	3.57%	0.459%

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ClientSampleId :
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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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.445	2603	2610	2627	rVB	48665	118137	3.26%	0.418%
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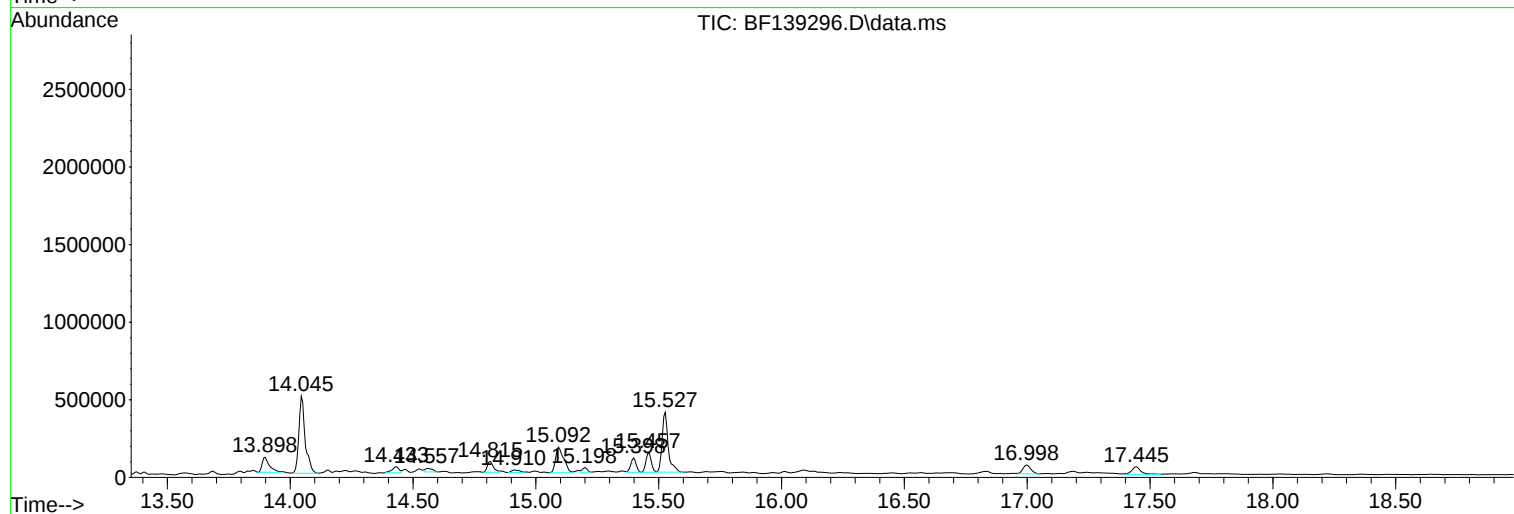
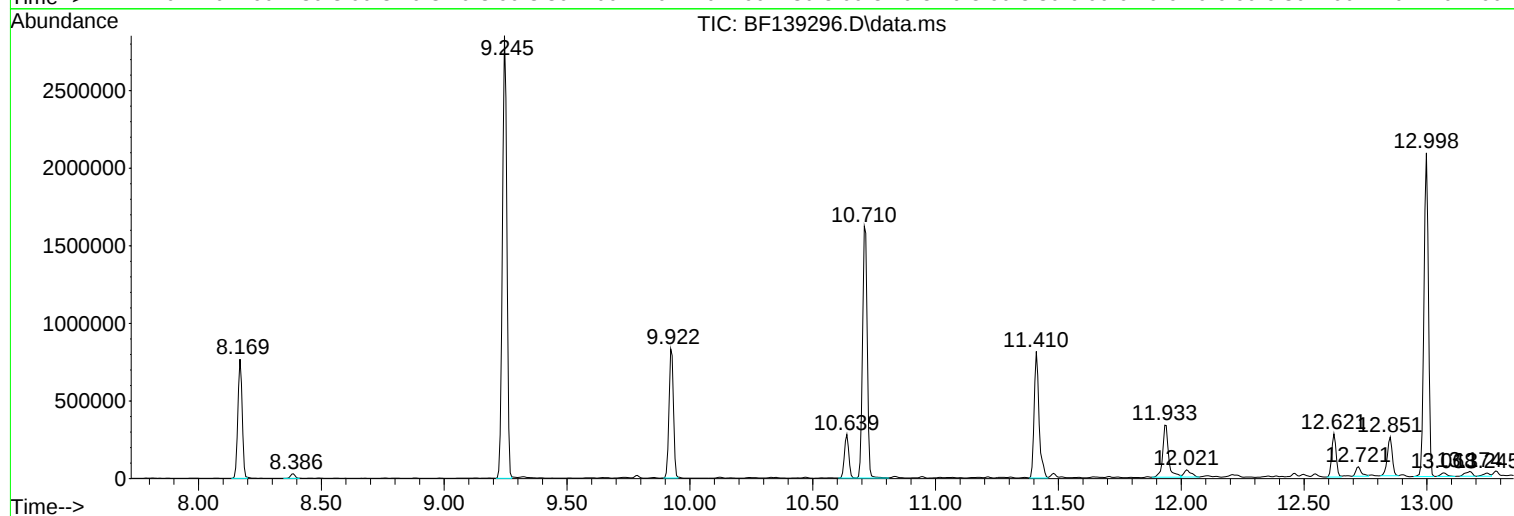
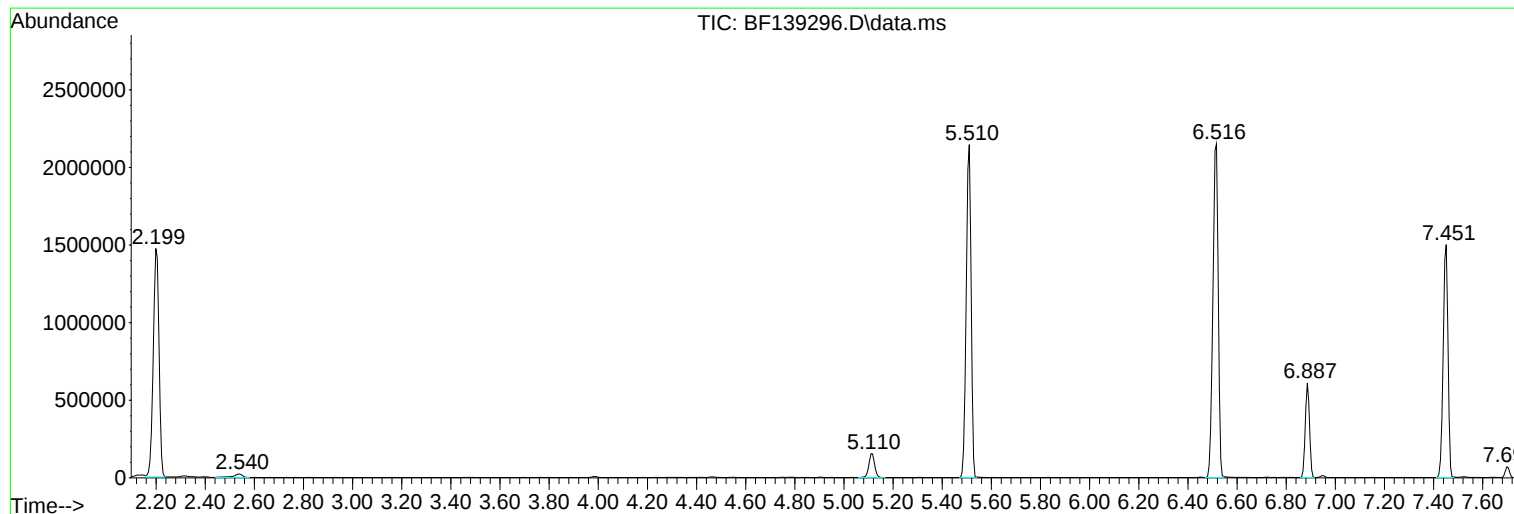
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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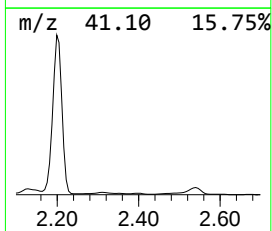
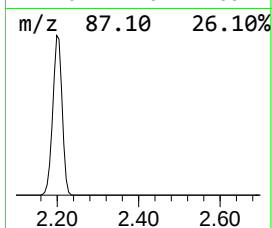
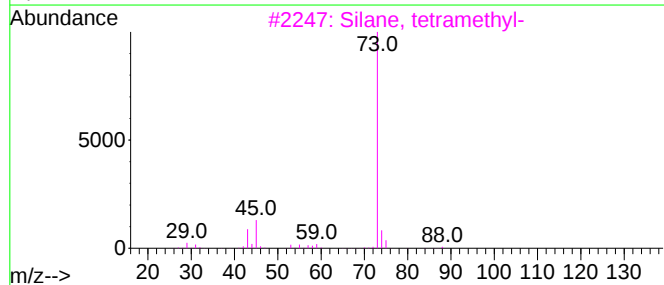
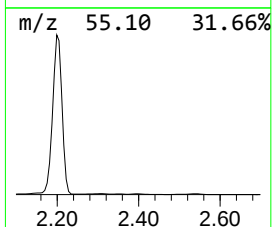
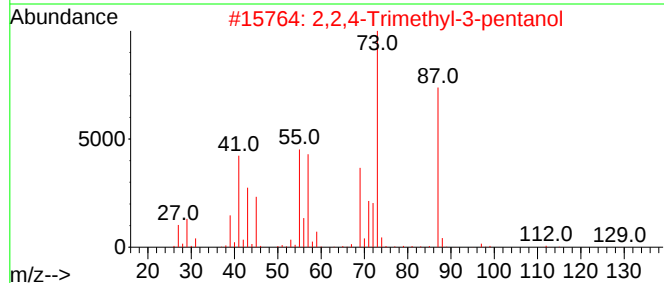
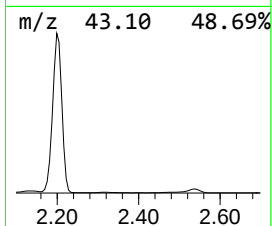
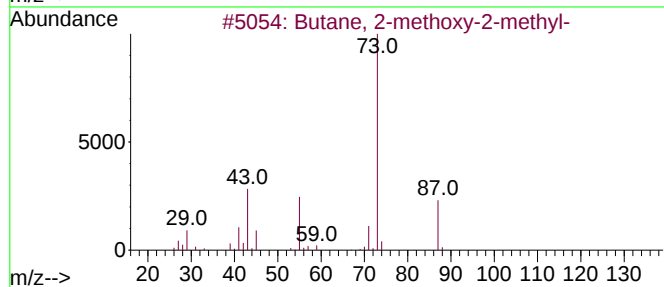
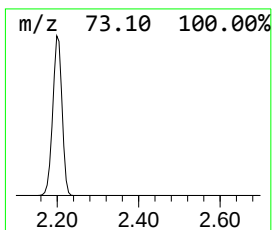
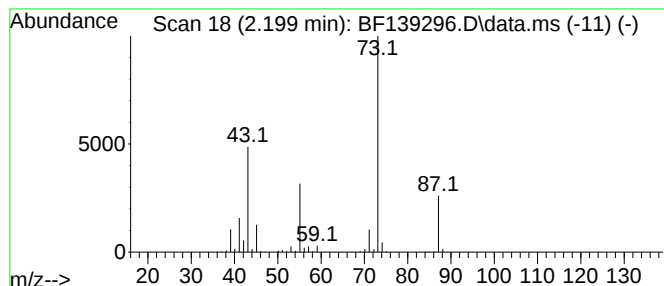
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.199	64.28 ng	2346310	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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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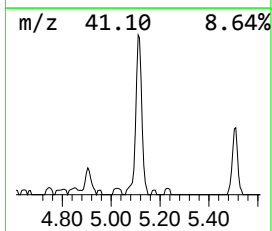
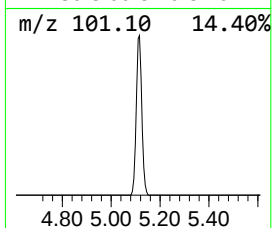
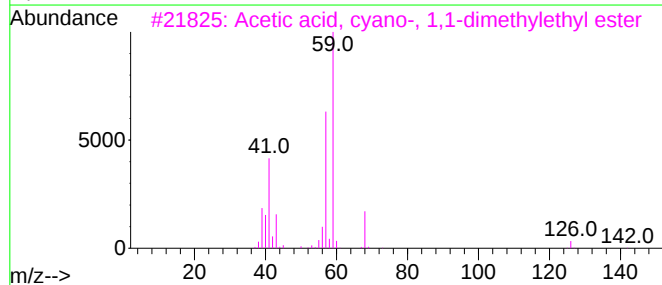
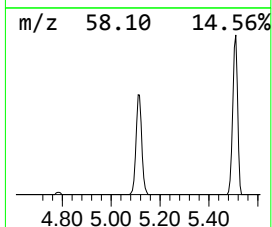
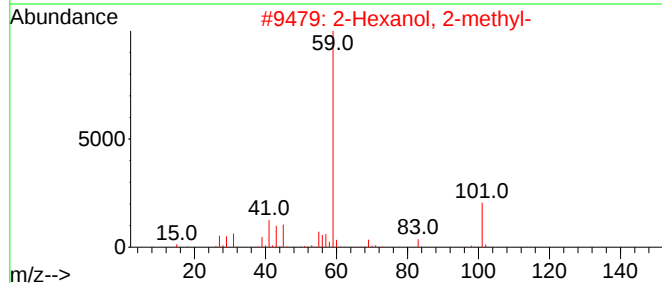
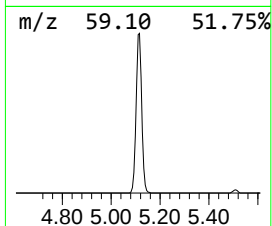
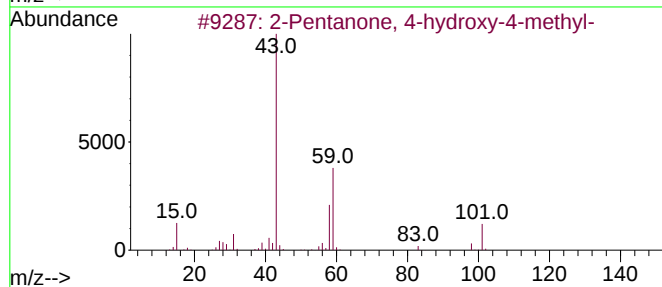
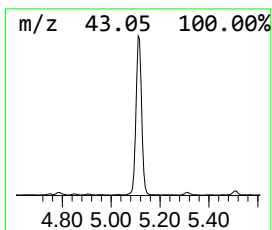
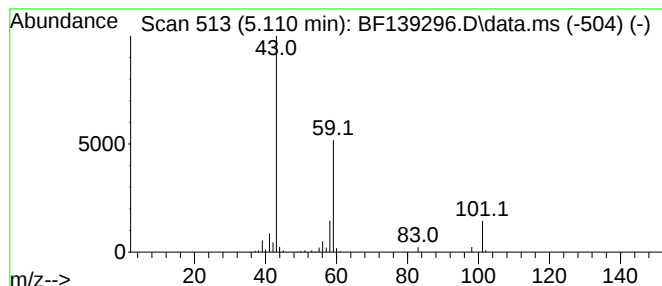
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	6.94 ng	253315	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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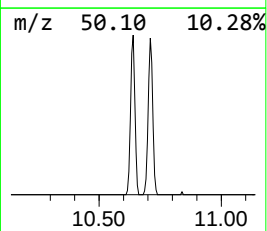
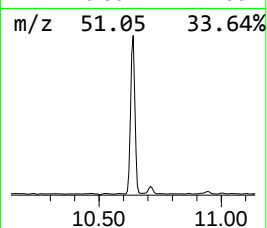
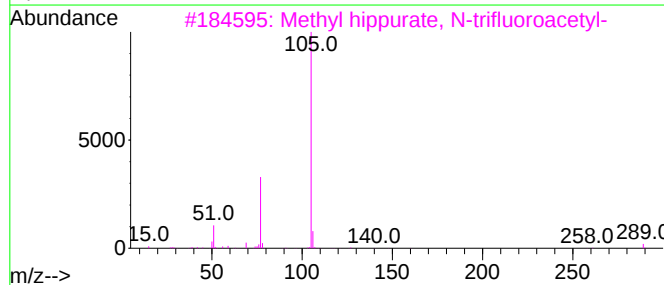
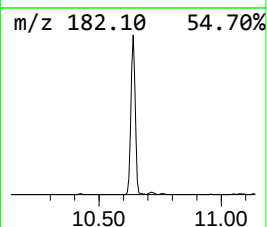
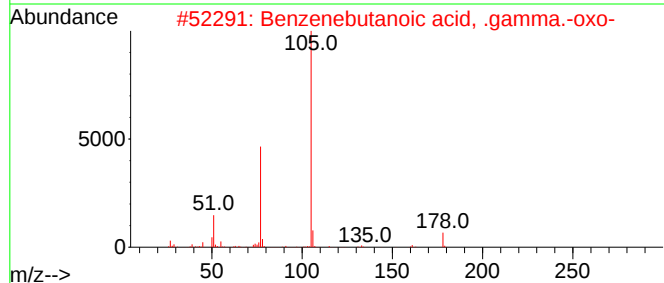
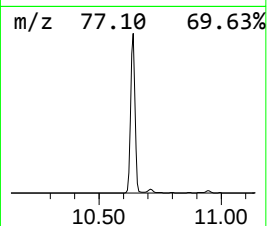
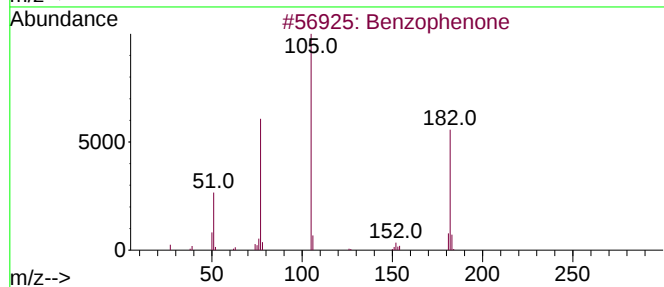
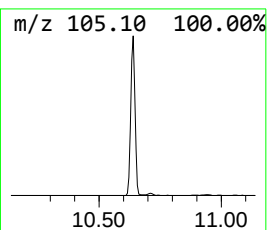
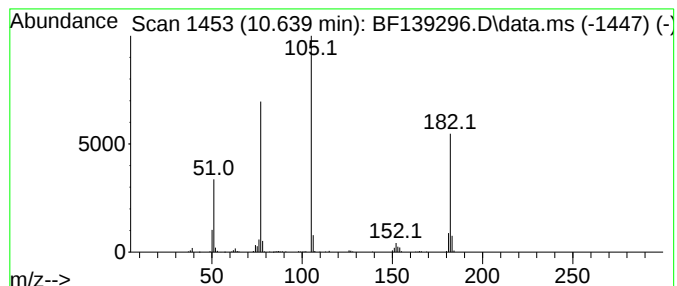
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	6.68 ng	346678	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
3			Methyl hippurate, N-trifluoroac...	289	C12H10F3NO4	073749-76-5	50
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50



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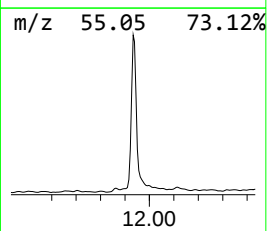
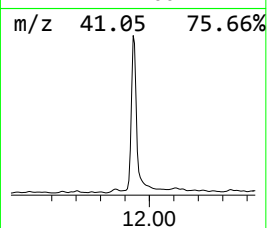
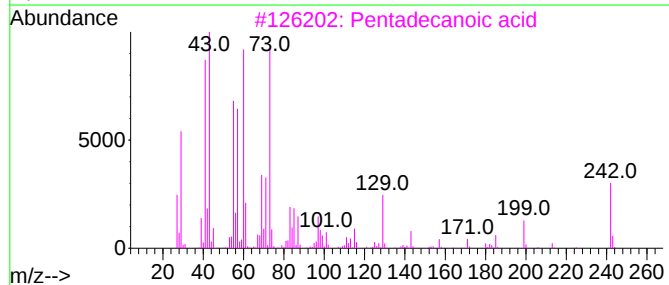
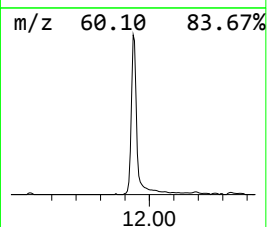
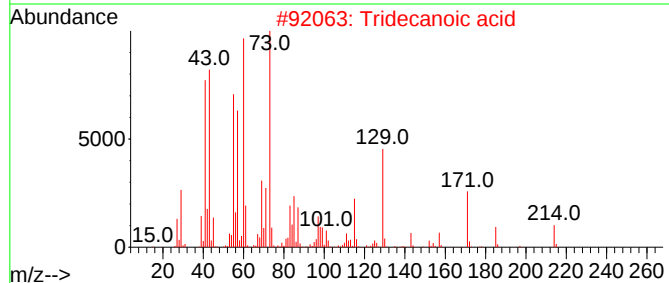
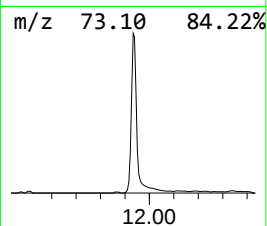
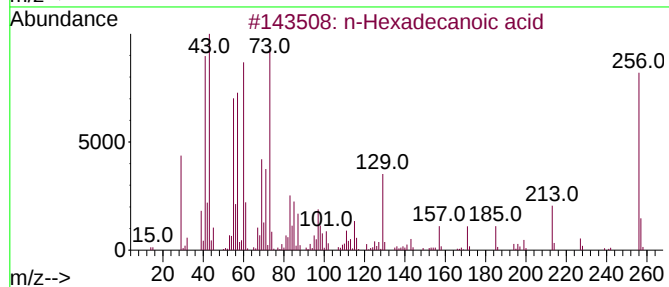
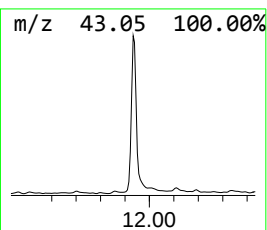
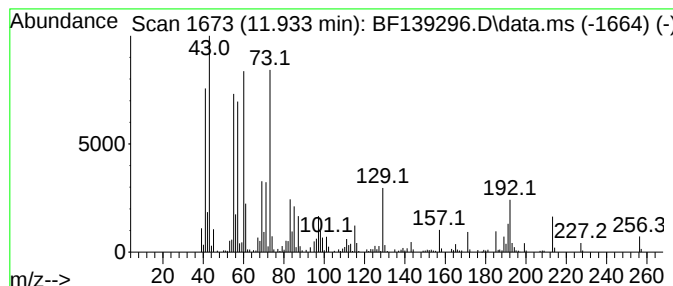
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.933	9.78 ng	552598	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	n-Decanoic acid		172	C10H20O2	000334-48-5	60



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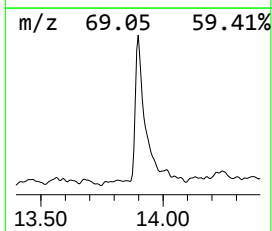
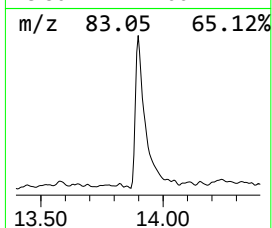
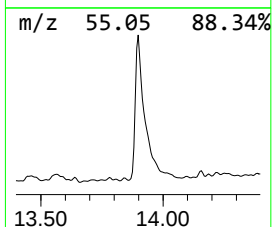
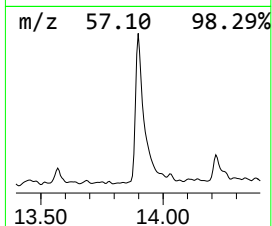
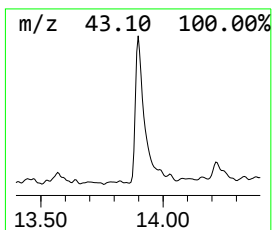
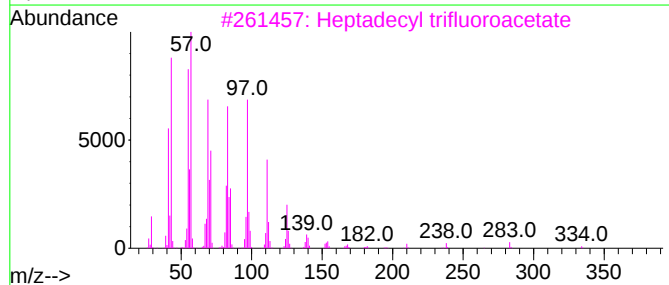
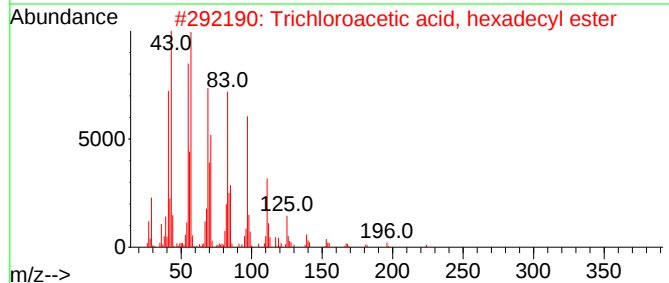
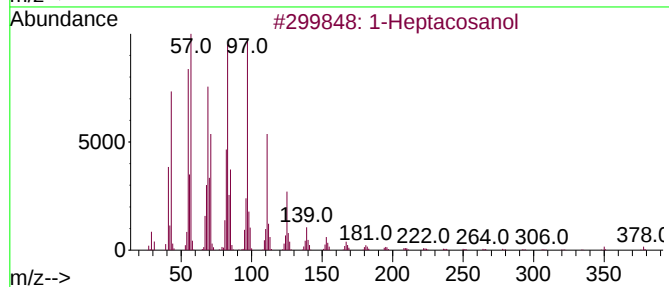
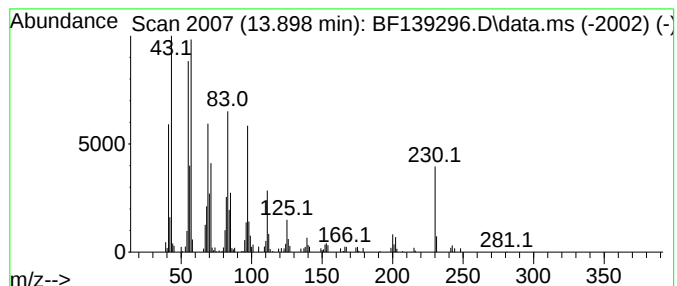
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	4.53 ng	201022	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139296.D
Acq On : 10 Sep 2024 13:30
Operator : RC/JU
Sample : P3905-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

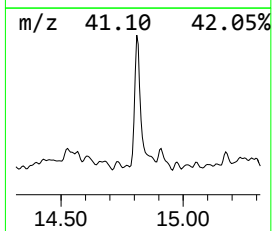
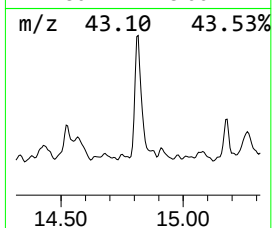
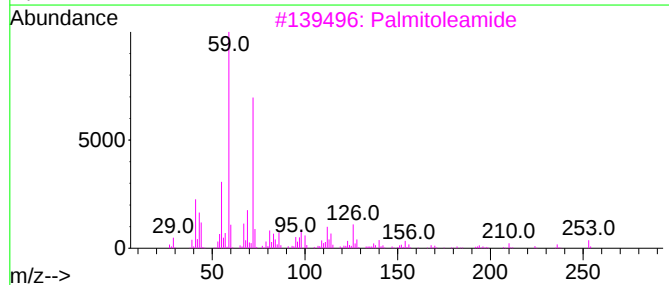
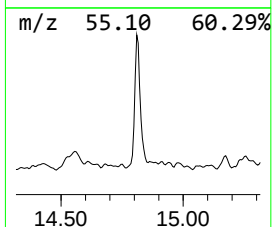
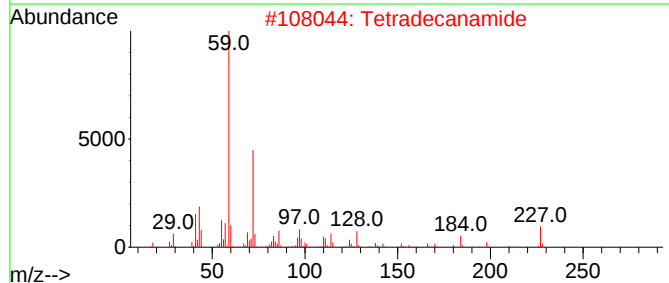
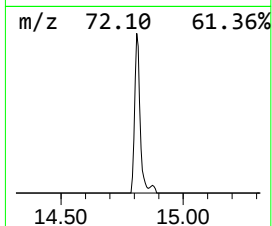
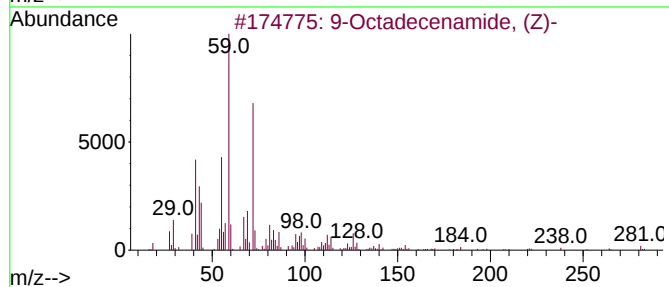
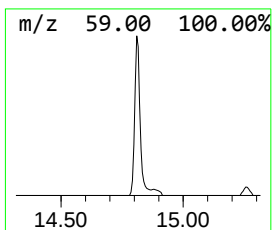
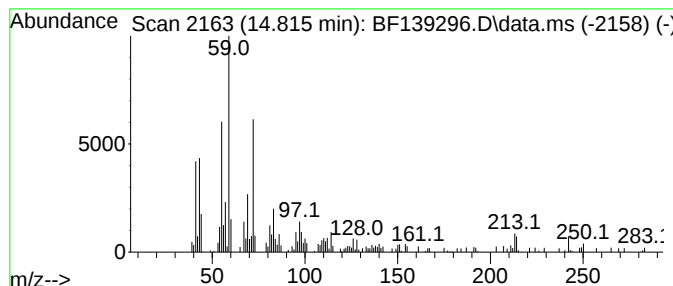
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	3.55 ng	117970	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
2			Tetradecanamide	227	C14H29NO	000638-58-4	59
3			Palmitoleamide	253	C16H31NO	106010-22-4	53
4			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50
5			N-Methyl-N-methoxycarbonylcarbam...	175	C6H9NO5	073830-21-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139296.D
Acq On : 10 Sep 2024 13:30
Operator : RC/JU
Sample : P3905-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

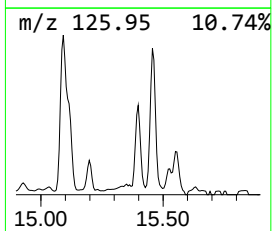
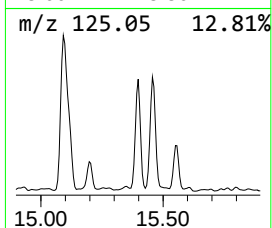
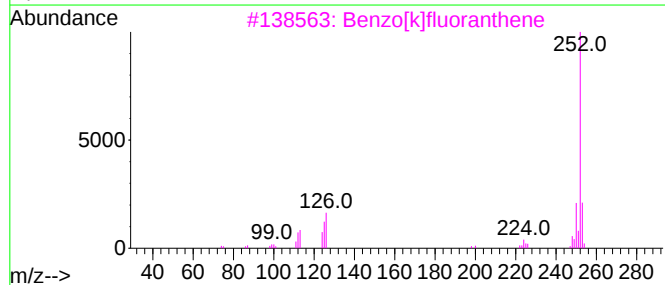
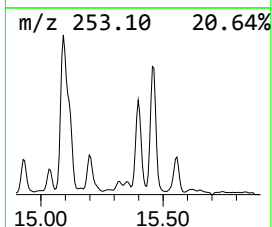
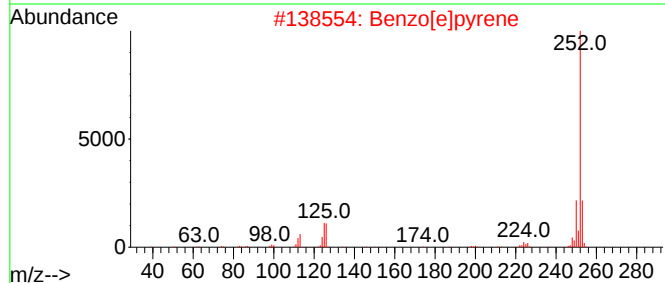
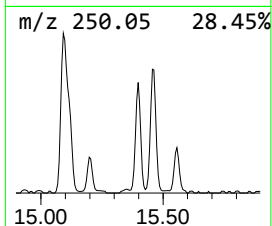
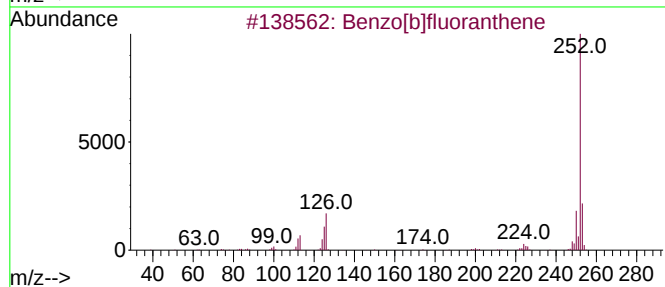
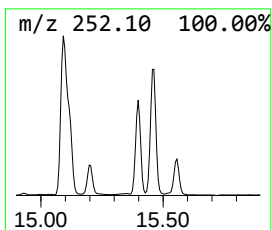
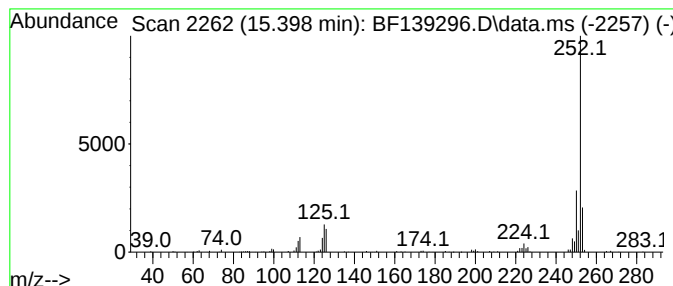
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	4.16 ng	138269	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
2			Benzo[e]pyrene	252	C20H12	000192-97-2	94
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Perylene	252	C20H12	000198-55-0	90
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139296.D
Acq On : 10 Sep 2024 13:30
Operator : RC/JU
Sample : P3905-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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...	2.199	64.3	ng	2346310	1	6.887	730012	20.0
2-Pentanone, 4-...	5.110	6.9	ng	253315	1	6.887	730012	20.0
Benzophenone	10.639	6.7	ng	346678	3	9.922	1038290	20.0
n-Hexadecanoic ...	11.933	9.8	ng	552598	4	11.410	1130360	20.0
1-Heptacosanol	13.898	4.5	ng	201022	5	14.045	887133	20.0
9-Octadecenamid...	14.815	3.5	ng	117970	6	15.527	665451	20.0
Benzo[e]pyrene	15.398	4.2	ng	138269	6	15.527	665451	20.0