

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022425\
 Data File : BF141737.D
 Acq On : 24 Feb 2025 11:27
 Operator : RC/JU
 Sample : Q1397-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP8

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-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.404	557	563	583	rBV	1648885	2259565	42.84%	8.029%
2	6.422	730	736	765	rBV	1631537	2346549	44.48%	8.338%
3	6.781	791	797	804	rBV	383742	503939	9.55%	1.791%
4	7.345	887	893	903	rBV	1078245	1509736	28.62%	5.365%
5	7.604	932	937	949	rBV	33434	54828	1.04%	0.195%
6	8.057	1009	1014	1030	rVB	478584	677773	12.85%	2.408%
7	9.134	1191	1197	1207	rBV	2170779	2788942	52.87%	9.910%
8	9.810	1307	1312	1325	rVB	586666	760079	14.41%	2.701%
9	10.528	1428	1434	1441	rVB	288923	378336	7.17%	1.344%
10	10.604	1441	1447	1462	rVV	1090149	1461666	27.71%	5.194%
11	11.298	1560	1565	1573	rBV2	577123	928022	17.59%	3.298%
12	11.680	1626	1630	1639	rBV5	22275	60676	1.15%	0.216%
13	11.833	1647	1656	1666	rBV	1093580	2284081	43.30%	8.116%
14	12.510	1766	1771	1781	rBV	257175	457230	8.67%	1.625%
15	12.610	1782	1788	1800	rVV	479200	1001548	18.99%	3.559%
16	12.739	1804	1810	1827	rVV	230301	459279	8.71%	1.632%
17	12.880	1828	1834	1842	rVB	1907322	2530921	47.98%	8.993%
18	13.139	1868	1878	1891	rVB	2283605	5275000	100.00%	18.744%
19	13.474	1932	1935	1941	rVB2	32529	53056	1.01%	0.189%
20	13.580	1950	1953	1960	rVB2	30035	54702	1.04%	0.194%
21	13.792	1984	1989	1997	rBV4	25586	62738	1.19%	0.223%
22	13.933	2006	2013	2026	rVB2	440030	788281	14.94%	2.801%
23	14.045	2027	2032	2037	rBV2	50112	88907	1.69%	0.316%
24	14.533	2110	2115	2125	rVB2	43482	85392	1.62%	0.303%
25	14.963	2183	2188	2202	rBV2	101641	317046	6.01%	1.127%
26	15.257	2234	2238	2244	rVB	54275	80378	1.52%	0.286%
27	15.315	2244	2248	2253	rBV	73935	112713	2.14%	0.401%
28	15.380	2253	2259	2271	rVB	348717	599753	11.37%	2.131%
29	16.810	2497	2502	2508	rVB2	37550	69744	1.32%	0.248%
30	17.245	2570	2576	2586	rVB	33156	91744	1.74%	0.326%

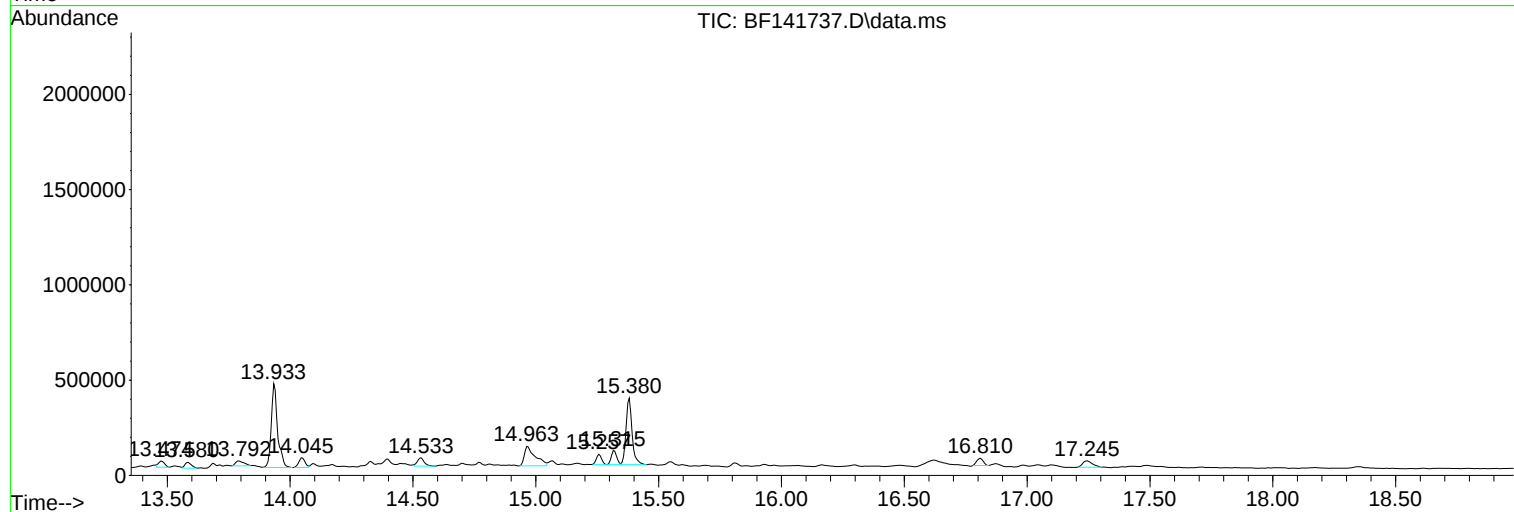
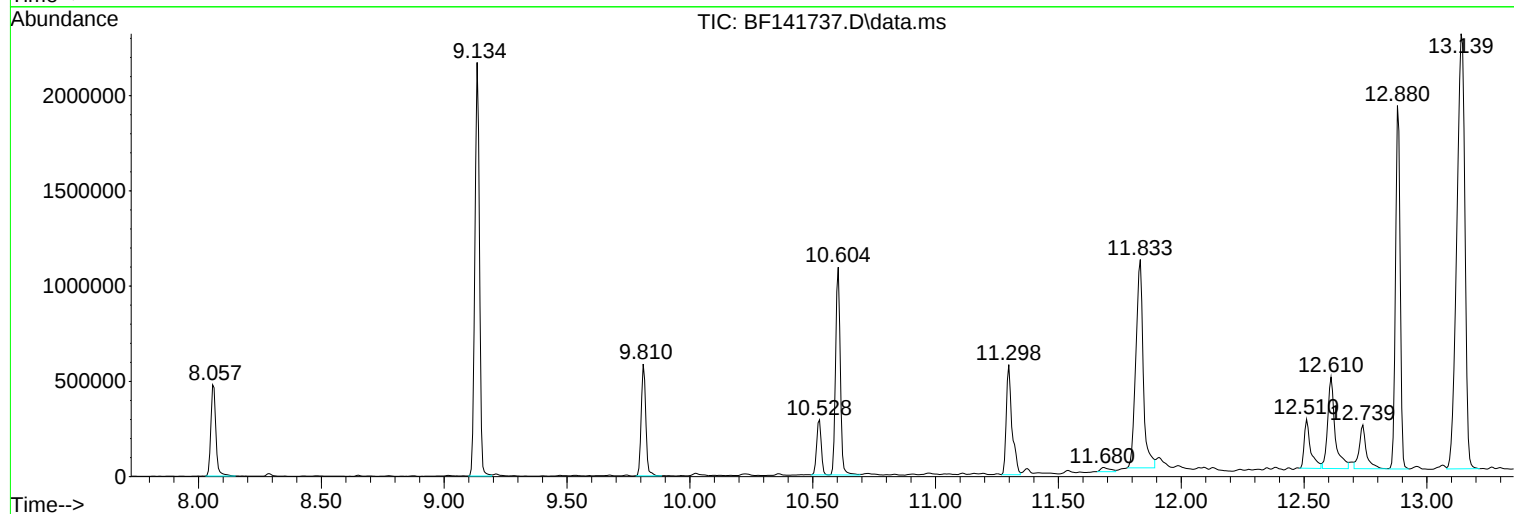
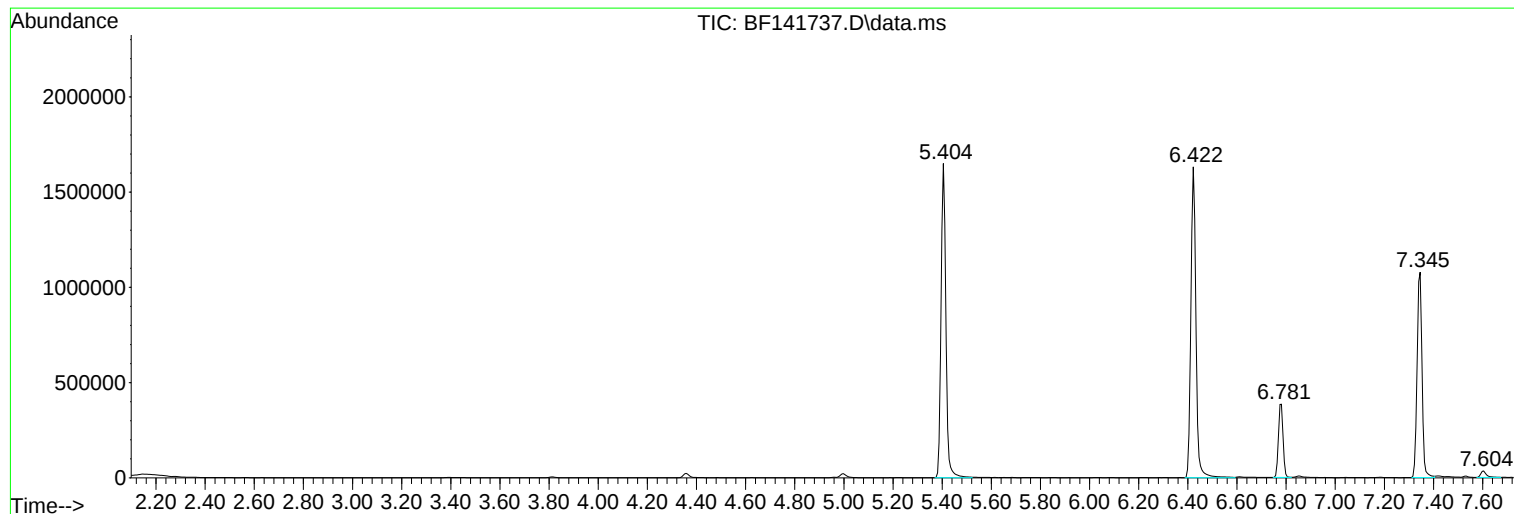
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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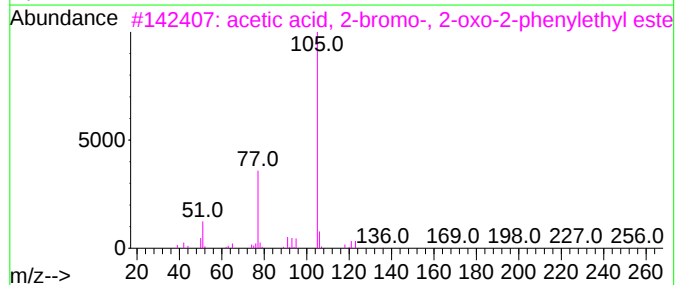
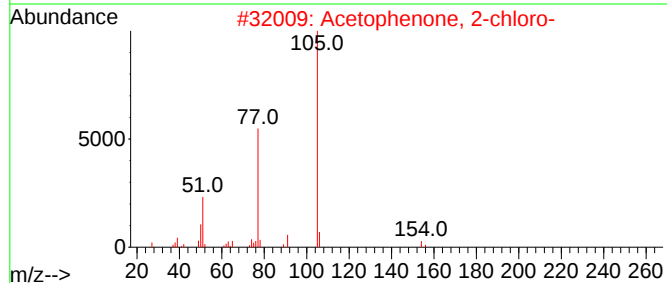
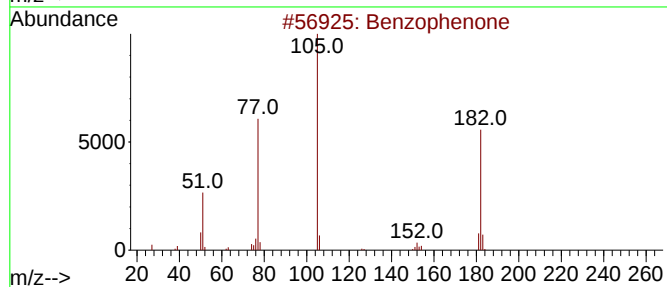
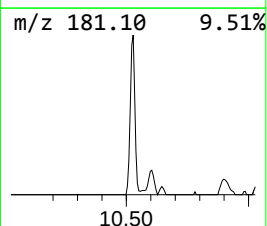
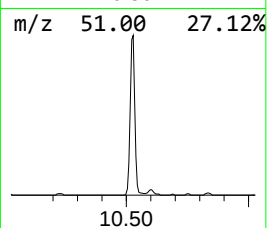
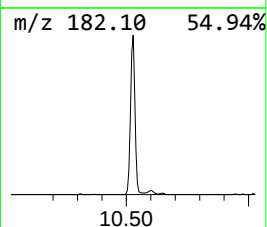
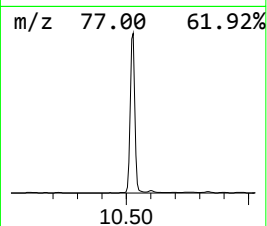
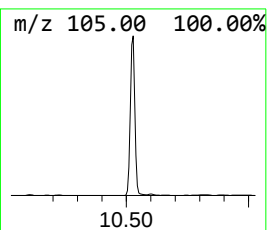
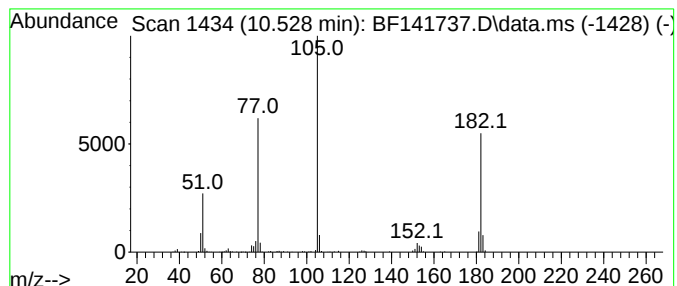
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.528	9.96 ng	378336	Acenaphthene-d10	9.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47



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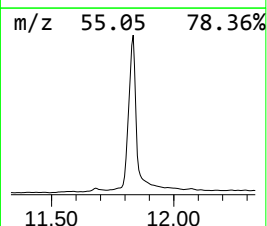
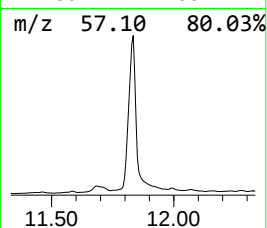
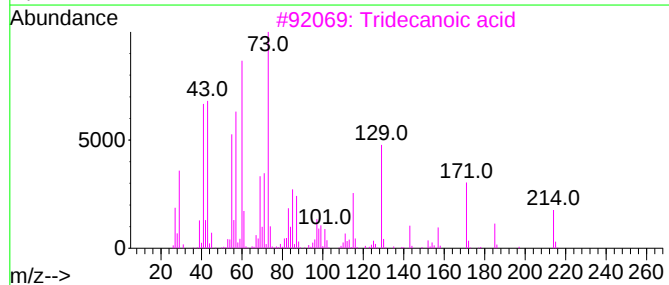
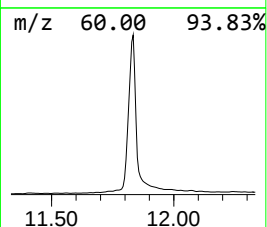
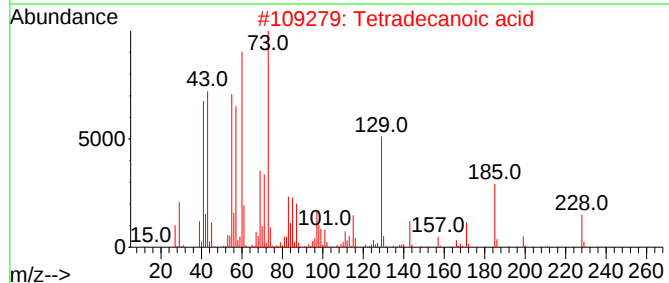
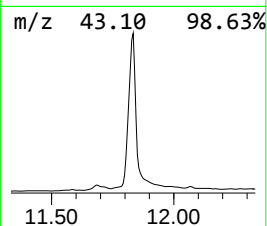
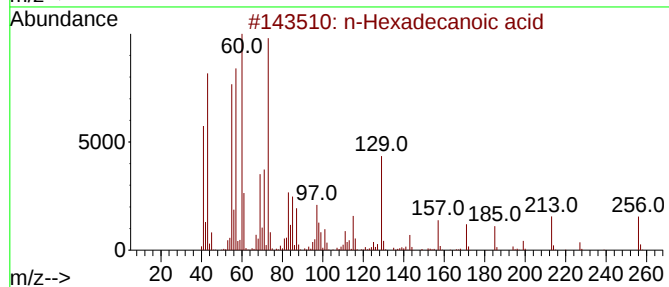
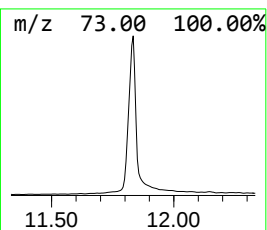
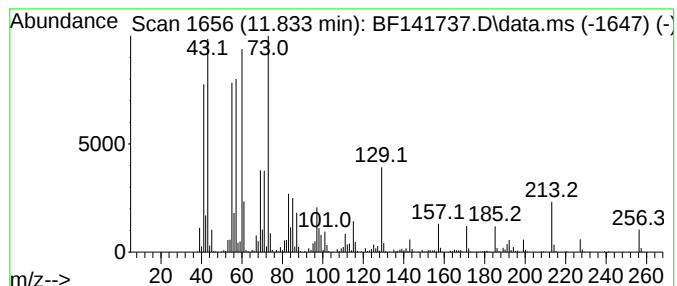
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	49.22 ng	2284080	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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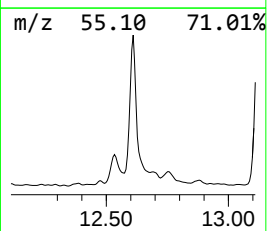
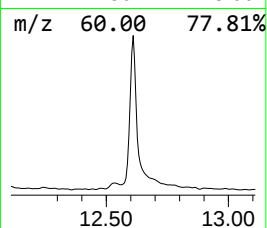
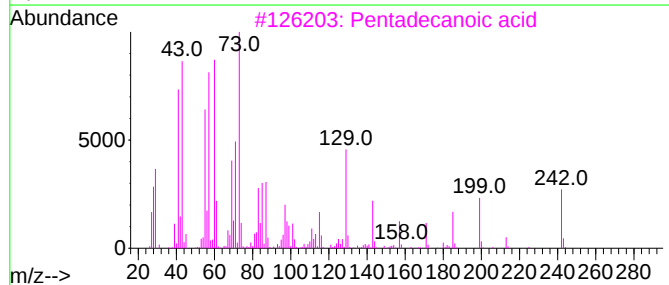
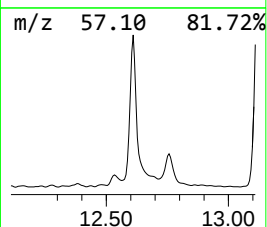
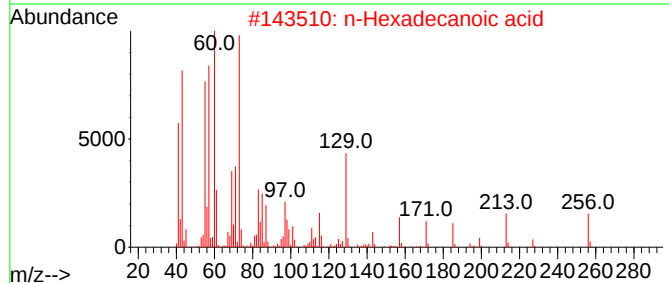
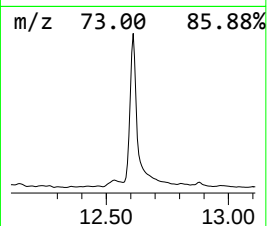
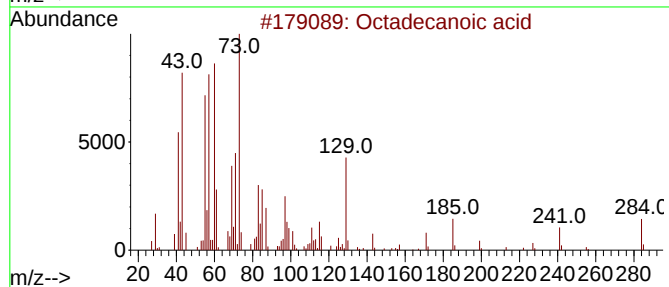
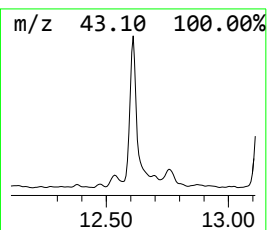
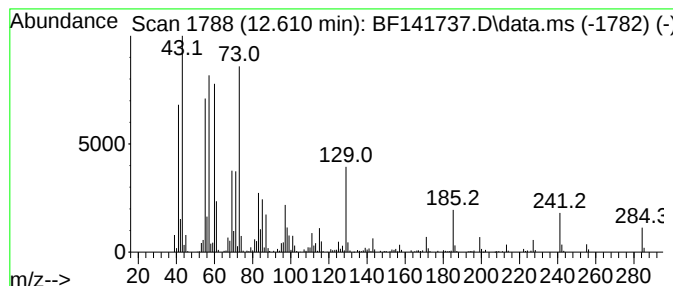
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	21.58 ng	1001550	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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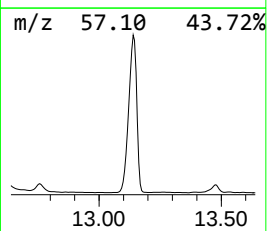
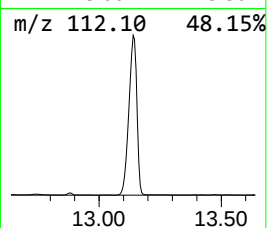
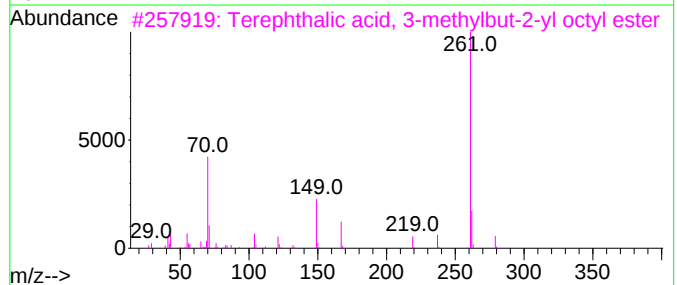
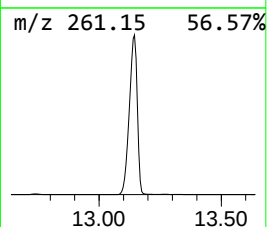
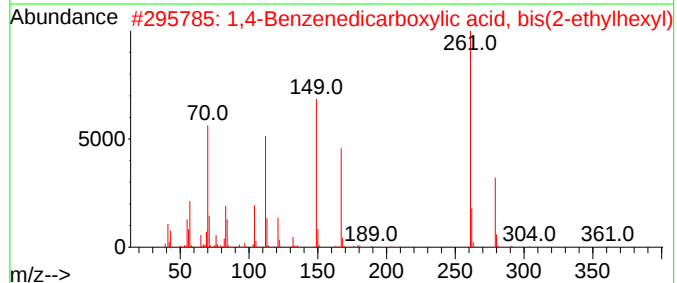
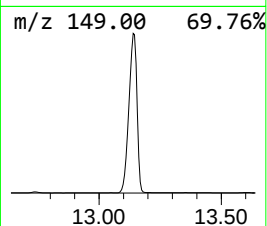
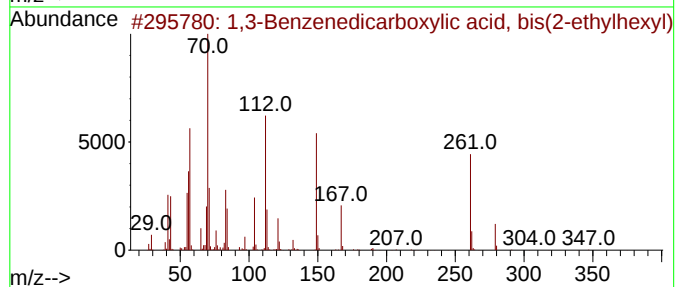
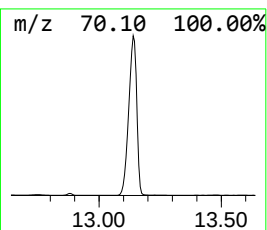
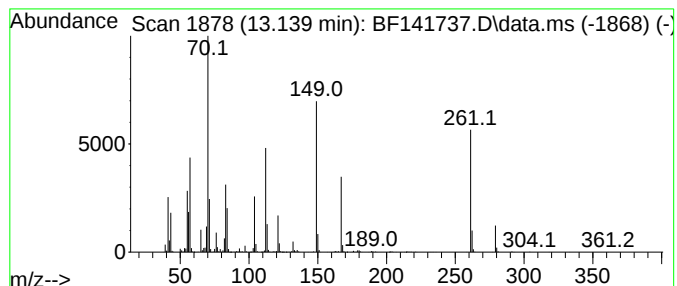
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Peak Number 4 1,3-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	133.84 ng	5275000	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	87
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
4			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	47
5			Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	35



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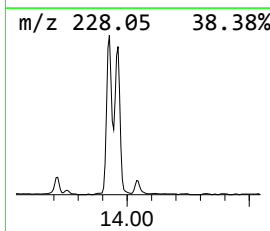
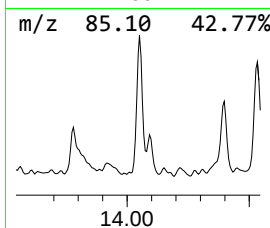
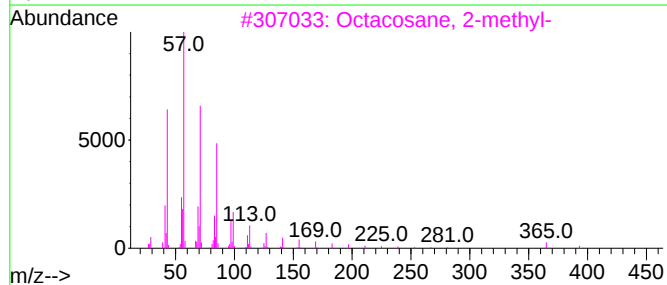
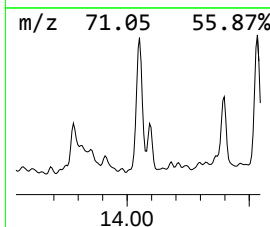
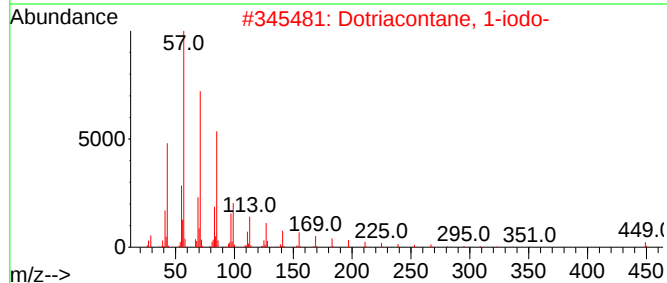
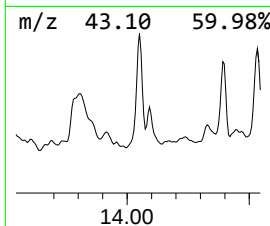
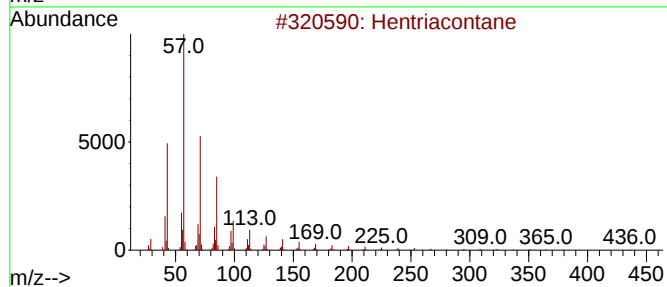
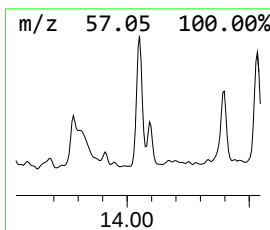
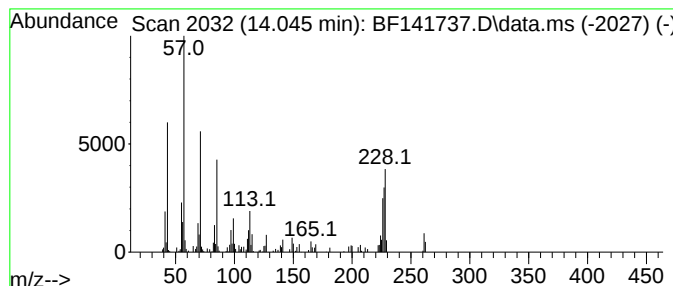
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Peak Number 5 unknown14.045 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.045	2.26 ng	88907	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	38
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	38
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	38
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	38
5			Pentacosane	352	C25H52	000629-99-2	38



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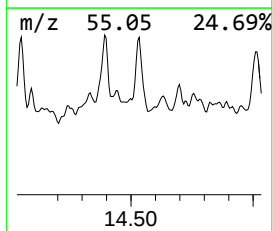
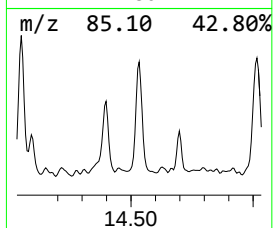
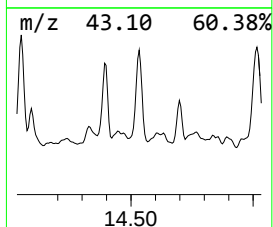
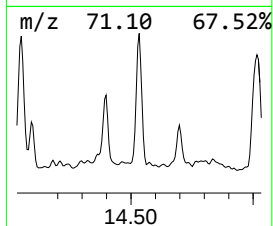
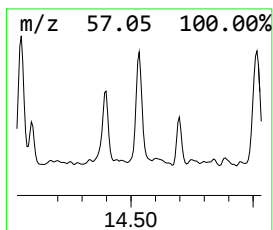
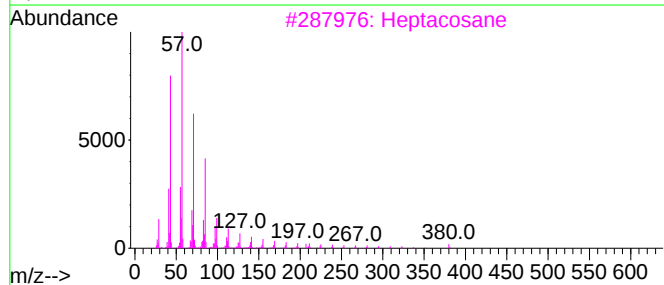
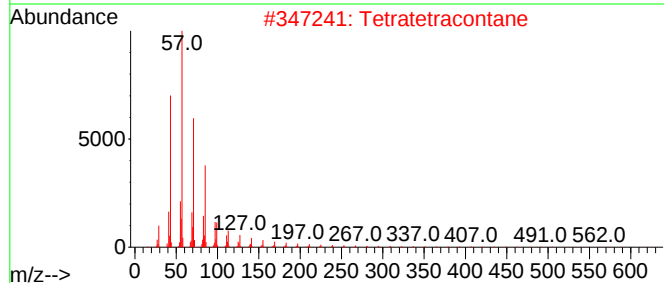
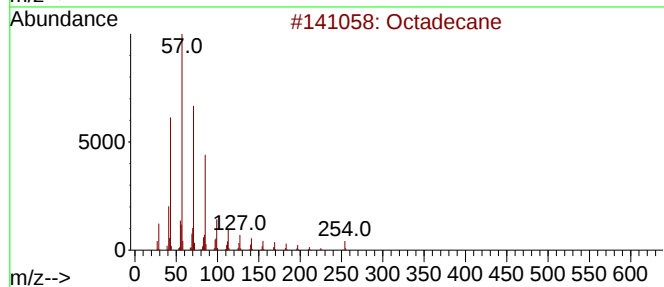
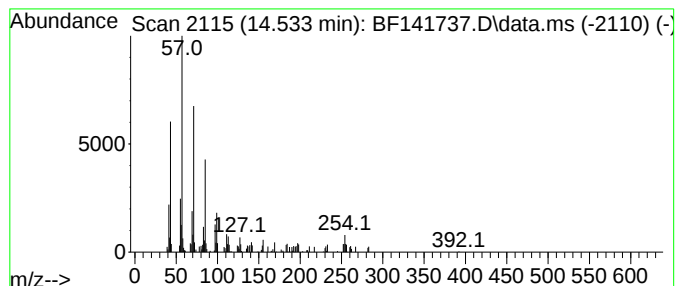
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	2.17 ng	85392	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	96
2			Tetratetracontane	619	C44H90	007098-22-8	76
3			Heptacosane	380	C27H56	000593-49-7	76
4			Eicosane	282	C20H42	000112-95-8	70
5			Tetradecane	198	C14H30	000629-59-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022425\
Data File : BF141737.D
Acq On : 24 Feb 2025 11:27
Operator : RC/JU
Sample : Q1397-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP8

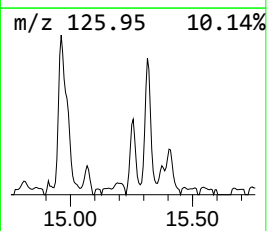
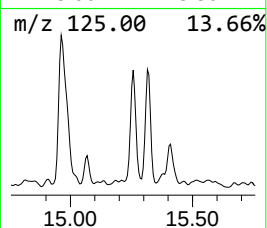
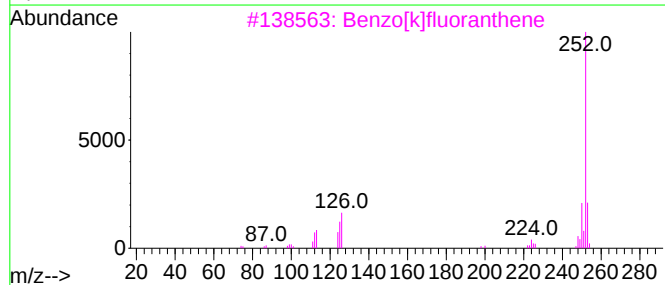
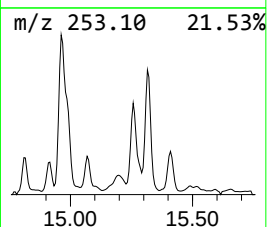
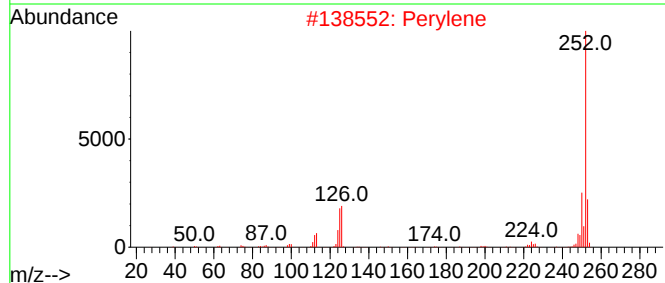
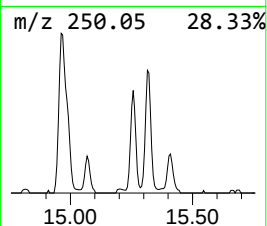
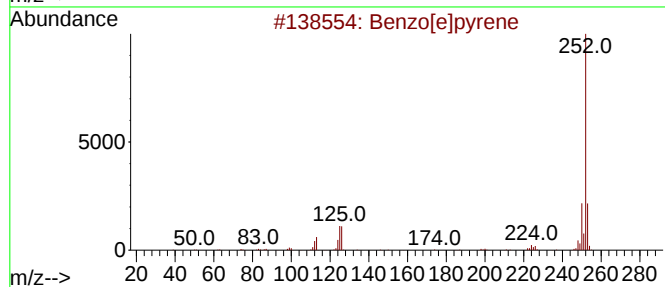
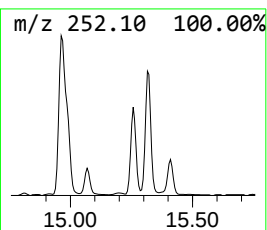
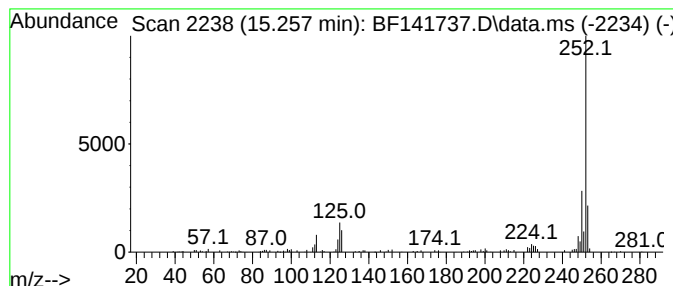
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.257	2.68 ng	80378	Perylene-d12	15.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Perylene	252	C20H12	000198-55-0	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022425\
Data File : BF141737.D
Acq On : 24 Feb 2025 11:27
Operator : RC/JU
Sample : Q1397-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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
Benzophenone	10.528	10.0	ng	378336	3	9.810	760079	20.0
n-Hexadecanoic ...	11.833	49.2	ng	2284080	4	11.298	928022	20.0
Octadecanoic acid	12.610	21.6	ng	1001550	4	11.298	928022	20.0
1,3-Benzenedica...	13.139	133.8	ng	5275000	5	13.933	788281	20.0
unknown14.045	14.045	2.3	ng	88907	5	13.933	788281	20.0
Octadecane	14.533	2.2	ng	85392	5	13.933	788281	20.0
Benzo[e]pyrene	15.257	2.7	ng	80378	6	15.380	599753	20.0