

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010825\
 Data File : BF141092.D
 Acq On : 08 Jan 2025 18:57
 Operator : RC/JU
 Sample : Q1025-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GREENBROOK-COMP

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-BF122624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141092.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.269	195	200	216	rBV	16411	43645	1.04%	0.132%
2	5.040	491	501	510	rVB2	32521	62713	1.49%	0.189%
3	5.310	541	547	552	rVB	71582	92354	2.19%	0.279%
4	5.440	562	569	574	rBV	2798579	3853987	91.56%	11.635%
5	5.663	602	607	617	rVB	220228	284463	6.76%	0.859%
6	5.998	660	664	669	rVB	38422	46270	1.10%	0.140%
7	6.287	706	713	720	rBV	30564	43852	1.04%	0.132%
8	6.445	734	740	754	rBV	2873791	3979691	94.54%	12.014%
9	6.828	800	805	810	rVB	834656	1038738	24.68%	3.136%
10	7.386	893	900	905	rBV	1936738	2512865	59.70%	7.586%
11	7.639	939	943	954	rVB	72032	92198	2.19%	0.278%
12	8.110	1017	1023	1037	rBV	1065053	1401480	33.29%	4.231%
13	9.180	1199	1205	1215	rBV	3307359	4209370	100.00%	12.707%
14	9.857	1312	1320	1334	rVB	1164278	1506598	35.79%	4.548%
15	10.569	1436	1441	1448	rBV	418539	546542	12.98%	1.650%
16	10.645	1448	1454	1471	rVV	2041888	2683064	63.74%	8.100%
17	10.769	1471	1475	1483	rVB3	30237	57811	1.37%	0.175%
18	11.345	1567	1573	1581	rBV2	1049982	1501860	35.68%	4.534%
19	11.874	1654	1663	1667	rBV	378781	591549	14.05%	1.786%
20	11.957	1673	1677	1685	rVB2	78651	157890	3.75%	0.477%
21	12.139	1703	1708	1719	rVB3	31225	76186	1.81%	0.230%
22	12.398	1748	1752	1755	rBV	41112	50395	1.20%	0.152%
23	12.557	1774	1779	1784	rBV	251474	340935	8.10%	1.029%
24	12.657	1792	1796	1802	rBV2	94537	159507	3.79%	0.482%
25	12.786	1812	1818	1824	rBV	288909	420921	10.00%	1.271%
26	12.933	1837	1843	1850	rVB	2428047	3227719	76.68%	9.744%
27	13.004	1851	1855	1862	rVV2	34183	55246	1.31%	0.167%
28	13.110	1867	1873	1877	rVB	48197	94051	2.23%	0.284%
29	13.216	1888	1891	1899	rVB	48396	66163	1.57%	0.200%
30	13.733	1974	1979	1982	rBV3	36744	71165	1.69%	0.215%
31	13.833	1992	1996	2006	rVB3	135456	224685	5.34%	0.678%
32	13.986	2016	2022	2032	rBV2	872793	1477805	35.11%	4.461%
33	14.474	2102	2105	2108	rBV3	61408	79337	1.88%	0.240%
34	15.033	2196	2200	2209	rVB	123182	278860	6.62%	0.842%
35	15.121	2211	2215	2223	rVB2	178354	273394	6.49%	0.825%
36	15.327	2247	2250	2255	rVB	76095	100543	2.39%	0.304%

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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-BF122624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.392	2257	2261	2266	rVV	101917	158515	3.77%	0.479%
38	15.457	2267	2272	2284	rVB	609668	1041870	24.75%	3.145%
39	15.939	2350	2354	2359	rBV	135806	221039	5.25%	0.667%

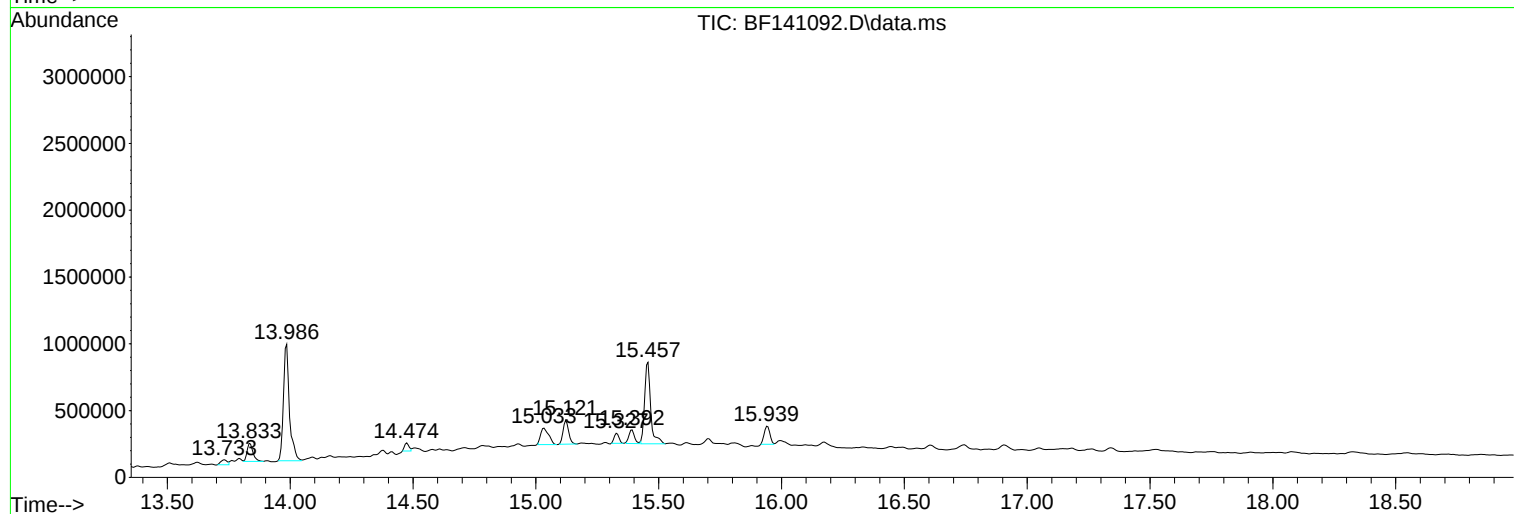
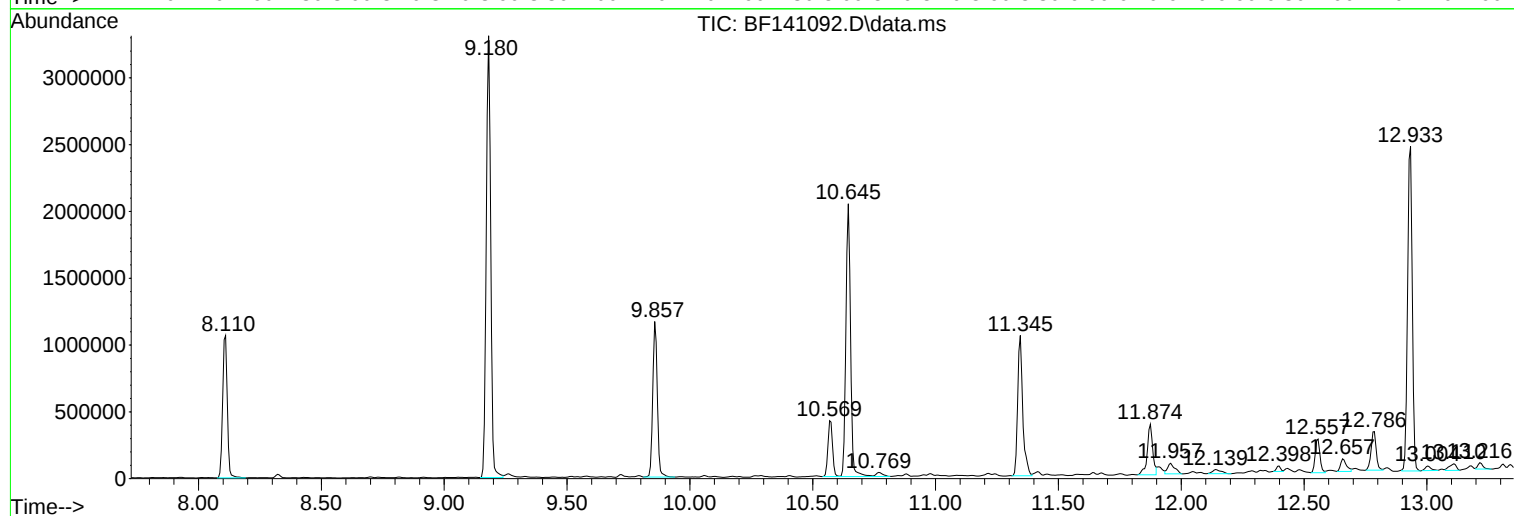
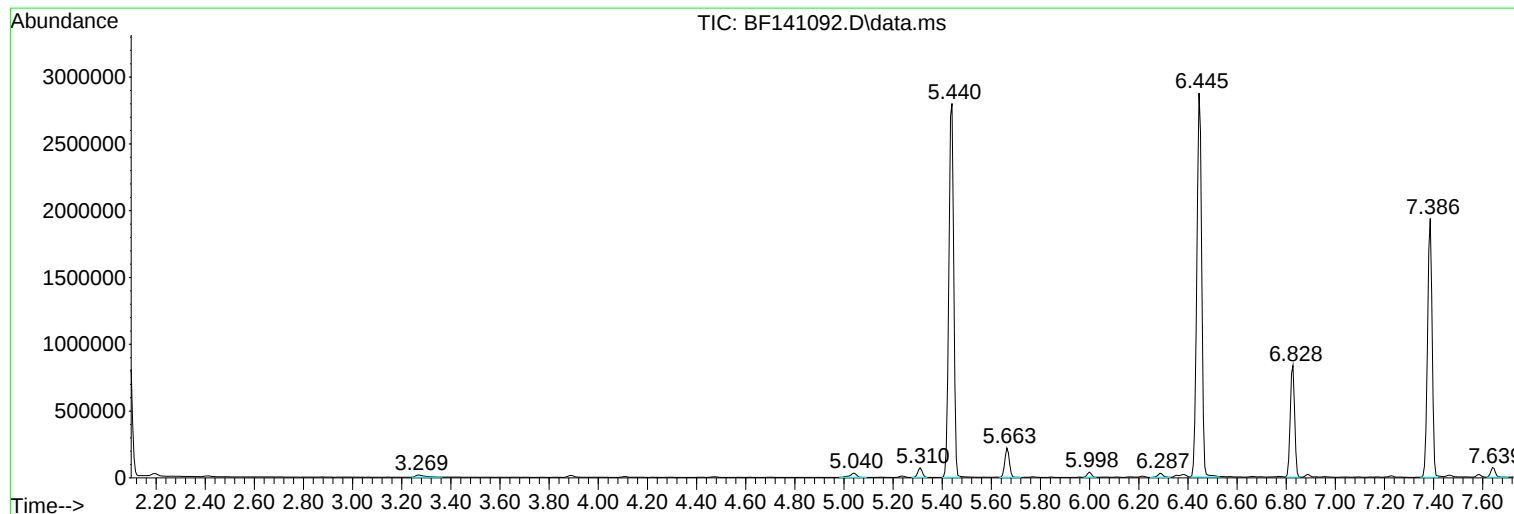
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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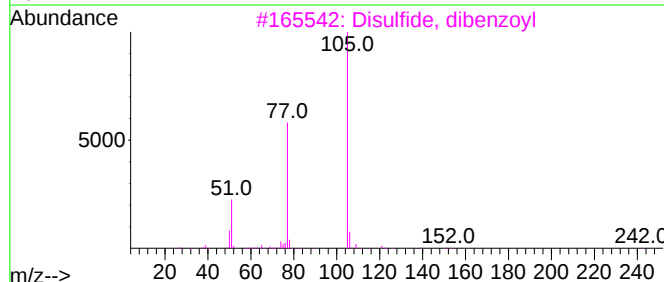
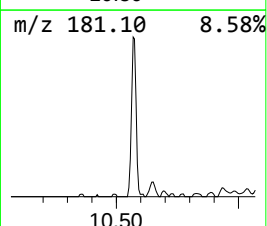
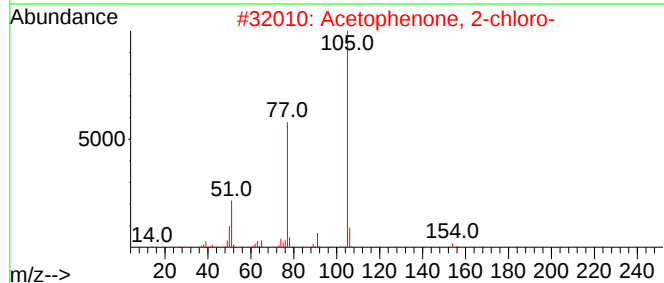
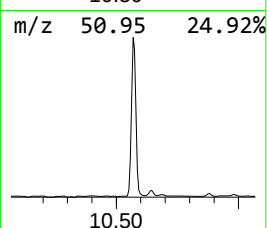
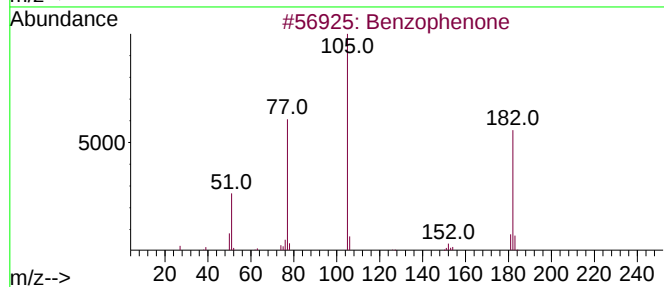
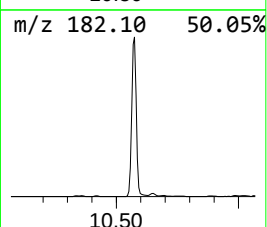
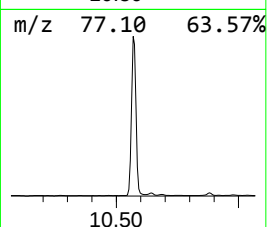
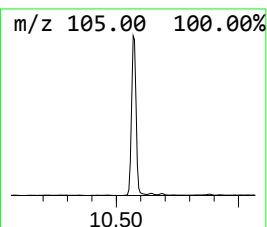
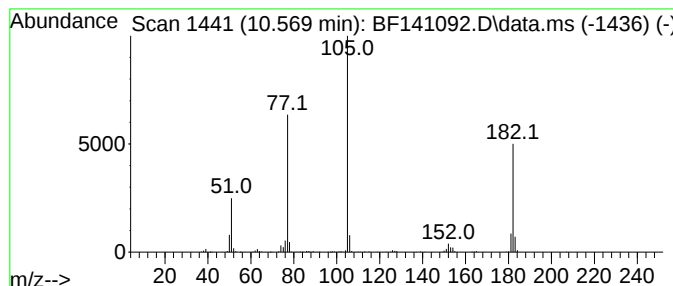
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	7.26 ng	546542	Acenaphthene-d10	9.857

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			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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Misc :
ALS Vial : 15 Sample Multiplier: 1

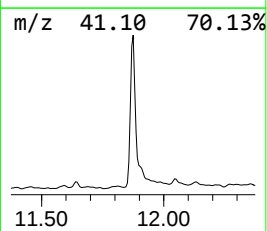
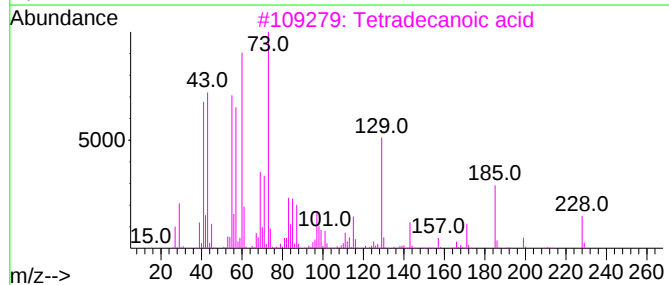
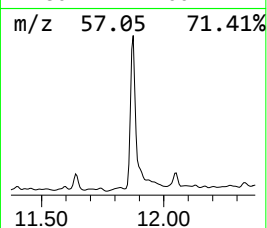
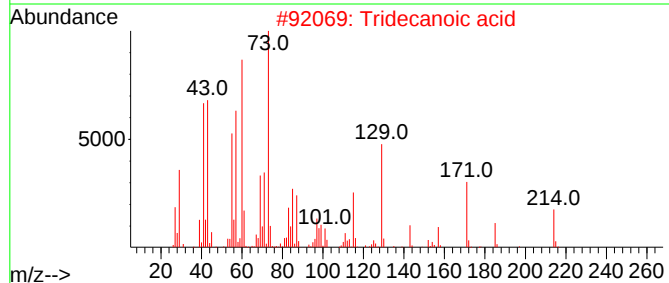
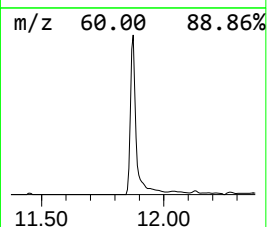
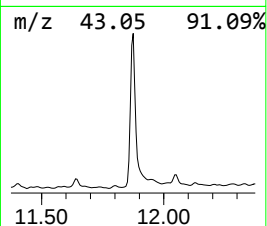
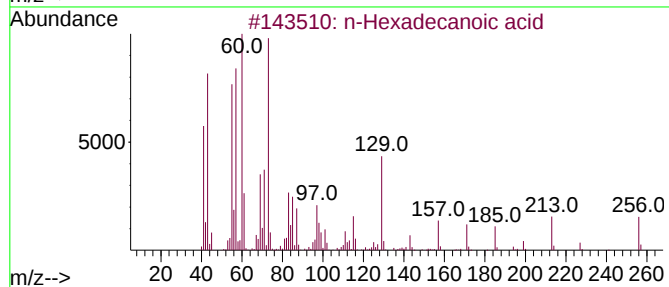
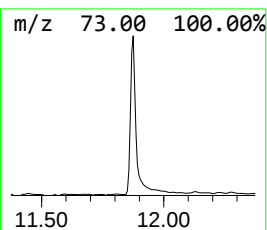
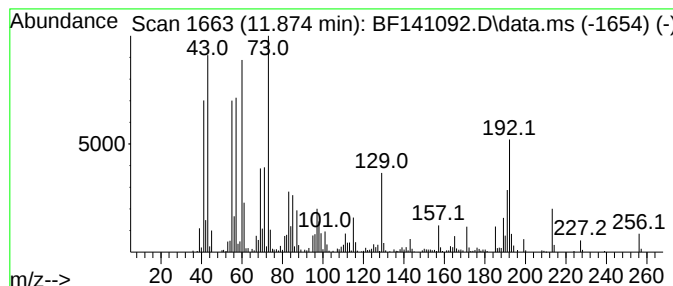
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.874	7.88 ng	591549	Phenanthrene-d10	11.345	
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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	92
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90



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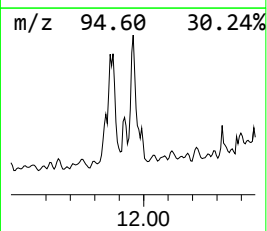
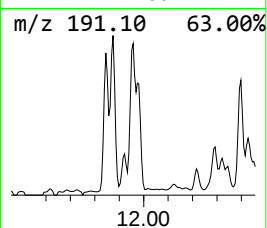
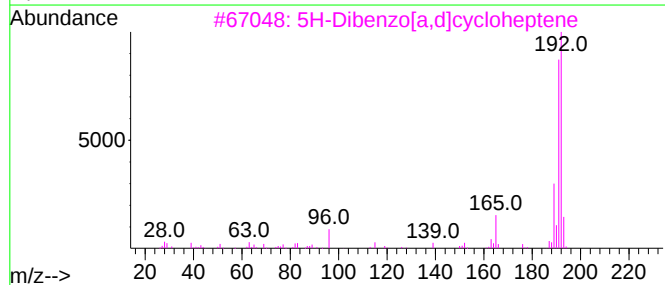
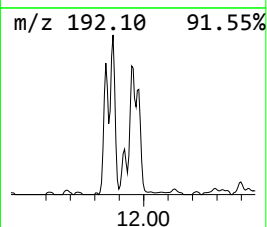
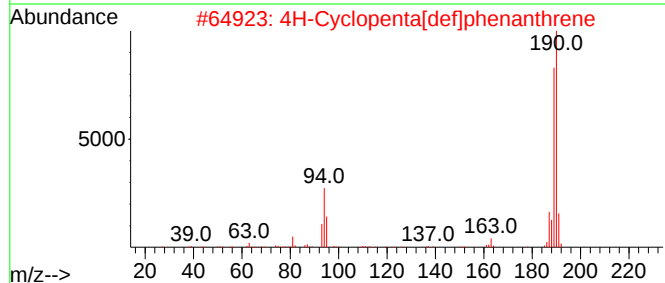
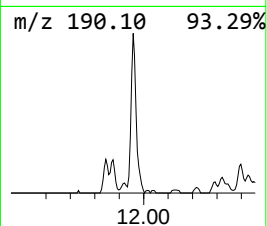
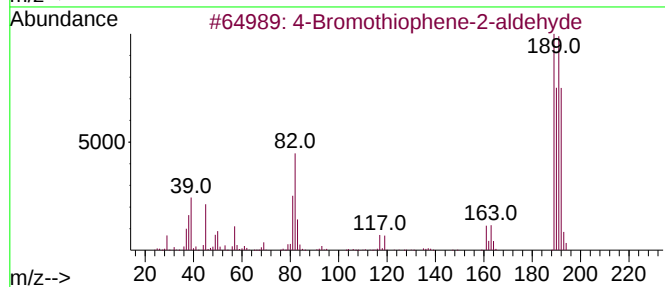
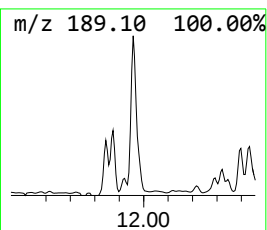
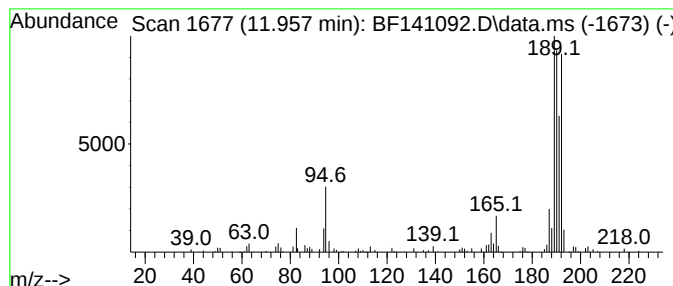
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4-Bromothiophene-2-aldehyde Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.957	2.10 ng	157890	Phenanthrene-d10	11.345	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	52
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	38
5	2-Bromo-4-fluorophenol	190	C6H4BrFO	000496-69-5	35



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Instrument :
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ClientSampleId :
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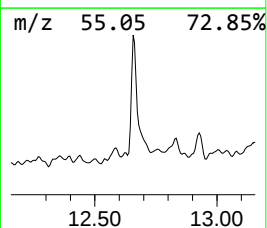
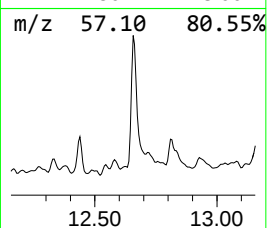
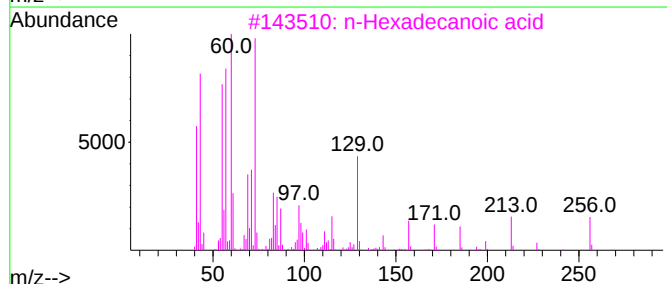
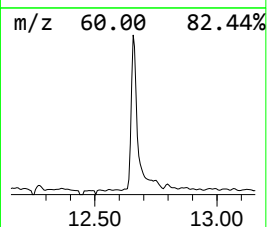
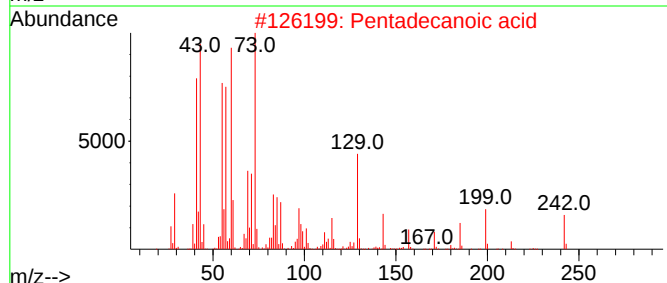
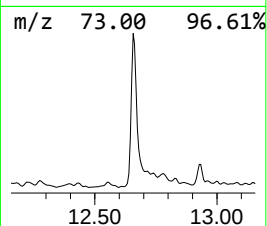
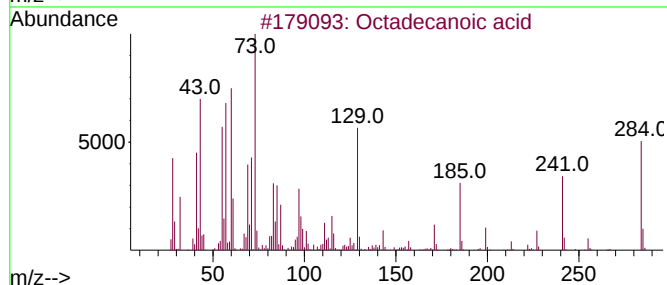
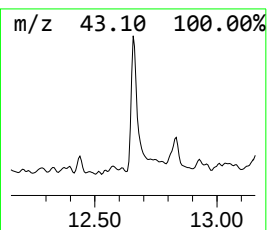
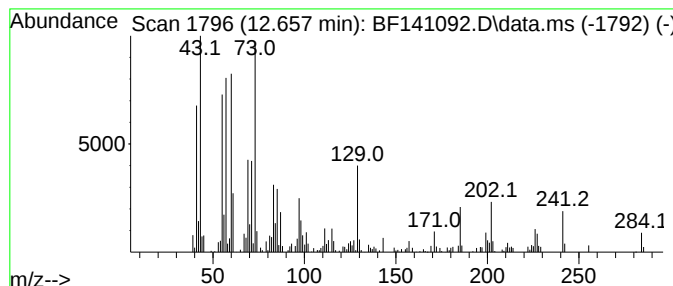
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	2.12 ng	159507	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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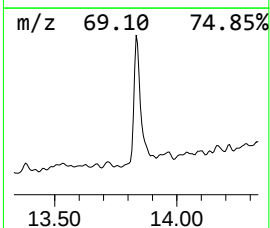
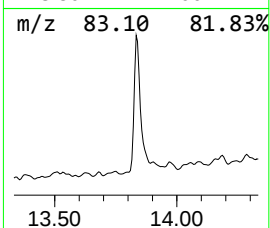
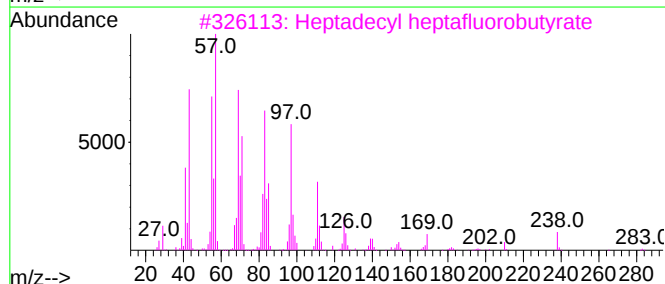
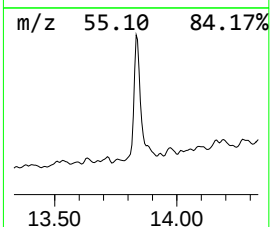
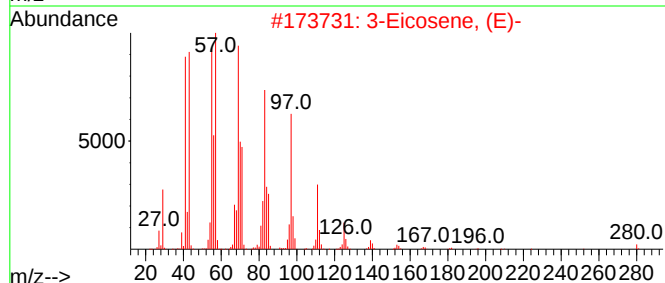
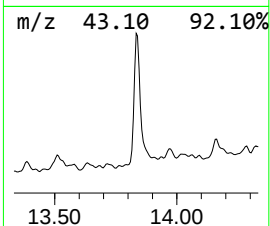
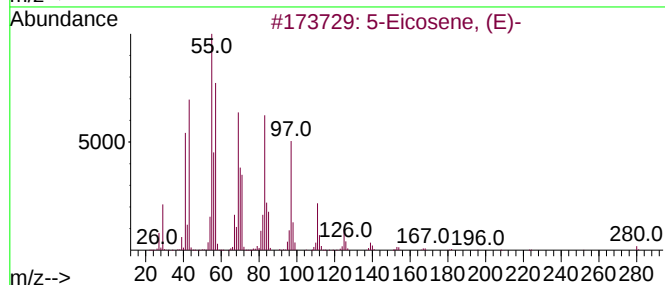
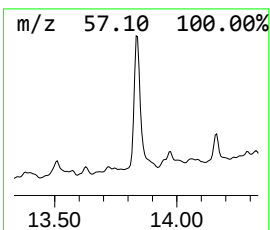
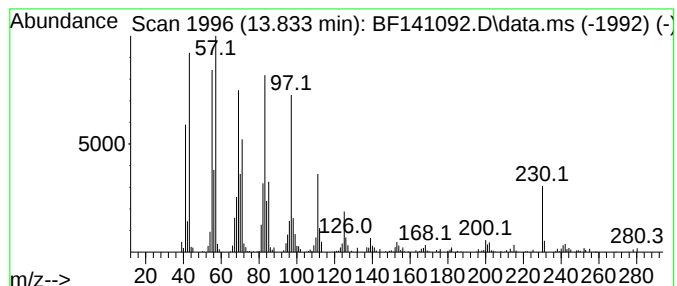
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	3.04 ng	224685	Chrysene-d12	13.986

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	97
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010825\
Data File : BF141092.D
Acq On : 08 Jan 2025 18:57
Operator : RC/JU
Sample : Q1025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GREENBROOK-COMP

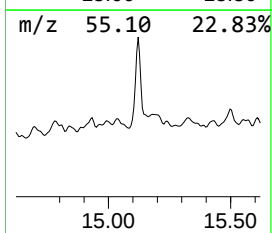
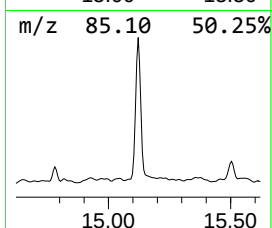
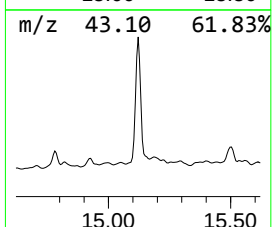
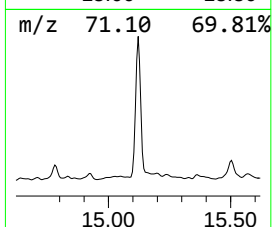
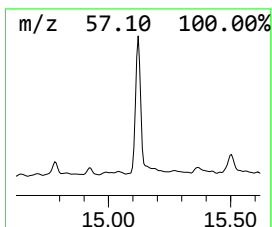
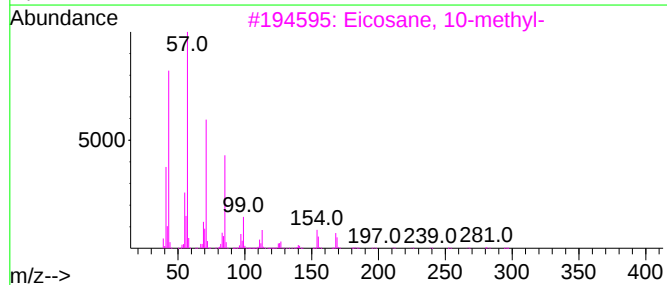
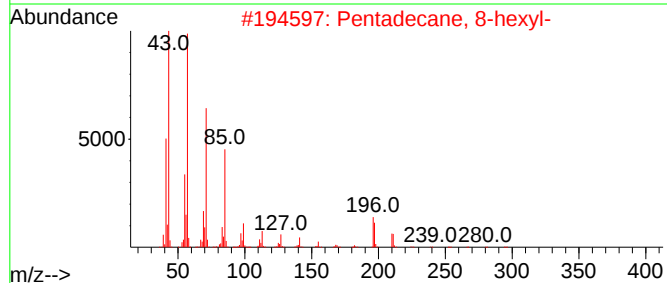
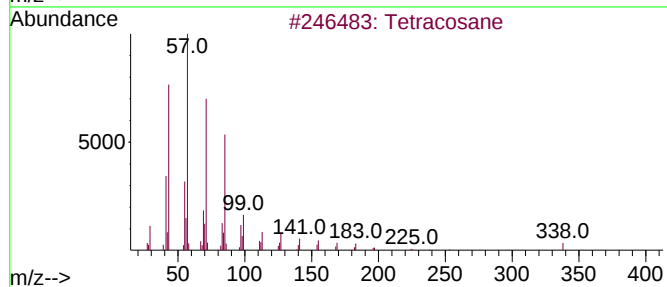
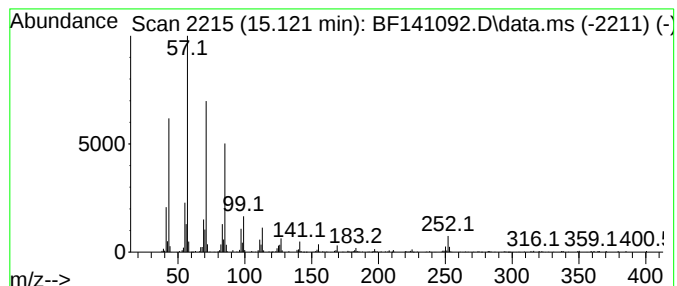
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	5.25 ng	273394	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	94
2			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
4			Octadecane	254	C18H38	000593-45-3	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010825\
Data File : BF141092.D
Acq On : 08 Jan 2025 18:57
Operator : RC/JU
Sample : Q1025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GREENBROOK-COMP

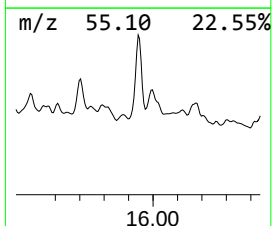
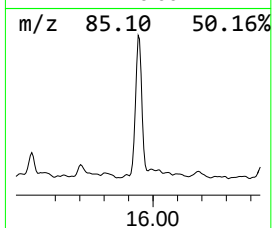
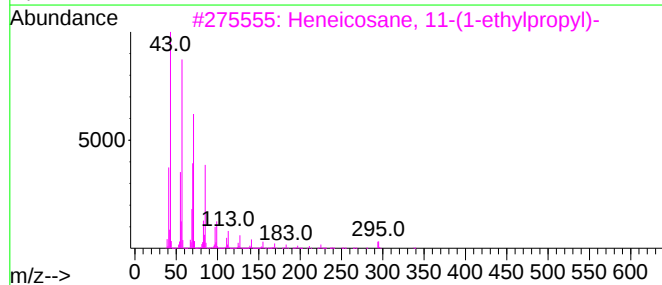
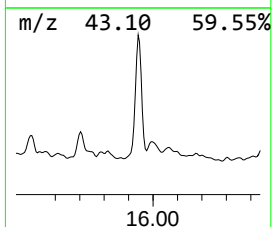
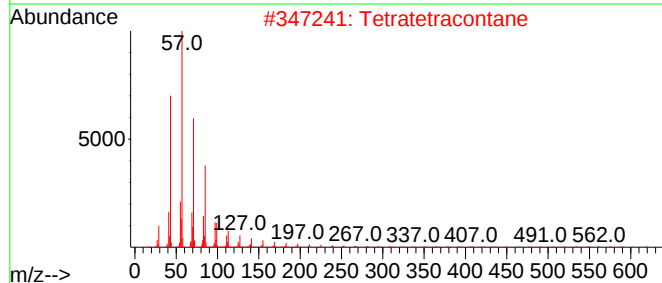
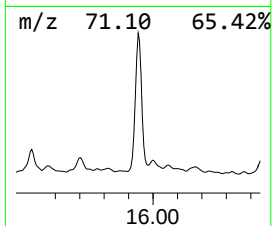
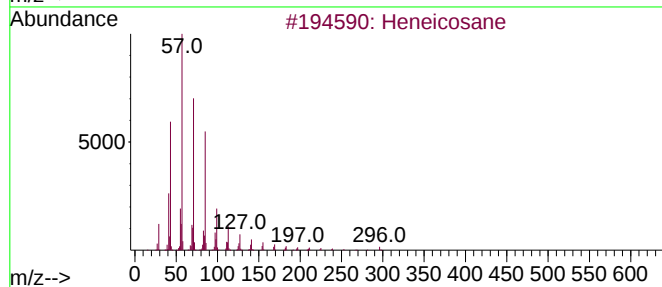
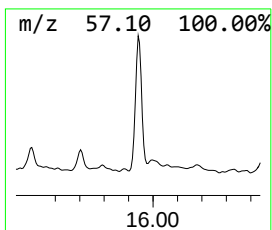
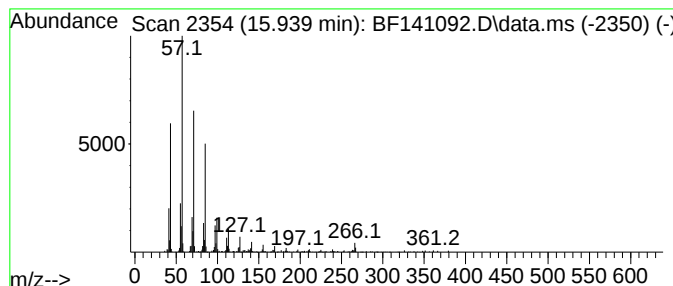
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	4.24 ng	221039	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
4			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
5			Triacontane	422	C30H62	000638-68-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010825\
Data File : BF141092.D
Acq On : 08 Jan 2025 18:57
Operator : RC/JU
Sample : Q1025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GREENBROOK-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.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	10.569	7.3	ng	546542	3	9.857	1506600	20.0
n-Hexadecanoic ...	11.874	7.9	ng	591549	4	11.345	1501860	20.0
4-Bromothiophen...	11.957	2.1	ng	157890	4	11.345	1501860	20.0
Octadecanoic acid	12.657	2.1	ng	159507	4	11.345	1501860	20.0
5-Eicosene, (E)-	13.833	3.0	ng	224685	5	13.986	1477810	20.0
Tetracosane	15.121	5.3	ng	273394	6	15.457	1041870	20.0
Heneicosane	15.939	4.2	ng	221039	6	15.457	1041870	20.0