

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081423\
 Data File : BF134758.D
 Acq On : 14 Aug 2023 14:26
 Operator : CG\JU
 Sample : 03989-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-PP24B

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134758.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	496	501	506	rVB	42997	53835	2.02%	0.240%
2	5.428	564	568	571	rBV	2730508	2519648	94.63%	11.238%
3	6.434	734	739	742	rBV	2630070	2450434	92.03%	10.929%
4	6.628	769	772	777	rBV	33897	38222	1.44%	0.170%
5	6.798	797	801	804	rBV	1184347	917413	34.46%	4.092%
6	7.357	891	896	899	rBV	1815875	1543277	57.96%	6.883%
7	8.075	1014	1018	1021	rBV	1437328	1145103	43.01%	5.107%
8	9.151	1197	1201	1212	rBV	3047839	2662598	100.00%	11.875%
9	9.275	1218	1222	1233	rVB	539718	562116	21.11%	2.507%
10	9.828	1313	1316	1320	rBV	1236610	1165197	43.76%	5.197%
11	10.028	1346	1350	1357	rBV	66044	100925	3.79%	0.450%
12	10.245	1383	1387	1396	rVB5	16096	29120	1.09%	0.130%
13	10.622	1447	1451	1454	rBV	1865533	1618669	60.79%	7.219%
14	10.739	1466	1471	1474	rBV5	37404	43918	1.65%	0.196%
15	10.975	1506	1511	1518	rBV6	16550	38360	1.44%	0.171%
16	11.322	1566	1570	1573	rBV	1326214	1138600	42.76%	5.078%
17	11.857	1655	1661	1678	rBV2	696646	892997	33.54%	3.983%
18	11.998	1682	1685	1690	rBV2	37571	45604	1.71%	0.203%
19	12.645	1790	1795	1807	rBV	237464	319069	11.98%	1.423%
20	12.739	1807	1811	1818	rVB4	28403	39705	1.49%	0.177%
21	12.916	1837	1841	1844	rBV	2706754	2391241	89.81%	10.665%
22	13.016	1853	1858	1865	rVB3	20273	37285	1.40%	0.166%
23	13.480	1934	1937	1948	rVB3	25146	47019	1.77%	0.210%
24	13.686	1967	1972	1979	rBV	30165	55083	2.07%	0.246%
25	13.786	1984	1989	1993	rVV6	17383	34755	1.31%	0.155%
26	13.827	1993	1996	2007	rVB	144670	219372	8.24%	0.978%
27	13.968	2015	2020	2031	rBV	946550	936949	35.19%	4.179%
28	14.221	2059	2063	2066	rBV2	32084	47286	1.78%	0.211%
29	14.686	2139	2142	2148	rVB3	42502	57515	2.16%	0.257%
30	14.763	2151	2155	2159	rVB	49692	54904	2.06%	0.245%
31	14.833	2163	2167	2172	rVV2	88776	109320	4.11%	0.488%
32	15.104	2209	2213	2218	rVB	68827	79396	2.98%	0.354%
33	15.186	2224	2227	2234	rVB2	31360	52113	1.96%	0.232%
34	15.439	2265	2270	2275	rBV	597394	771059	28.96%	3.439%
35	15.492	2276	2279	2287	rVB	80856	107261	4.03%	0.478%
36	15.945	2351	2356	2361	rVB2	62891	95880	3.60%	0.428%

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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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

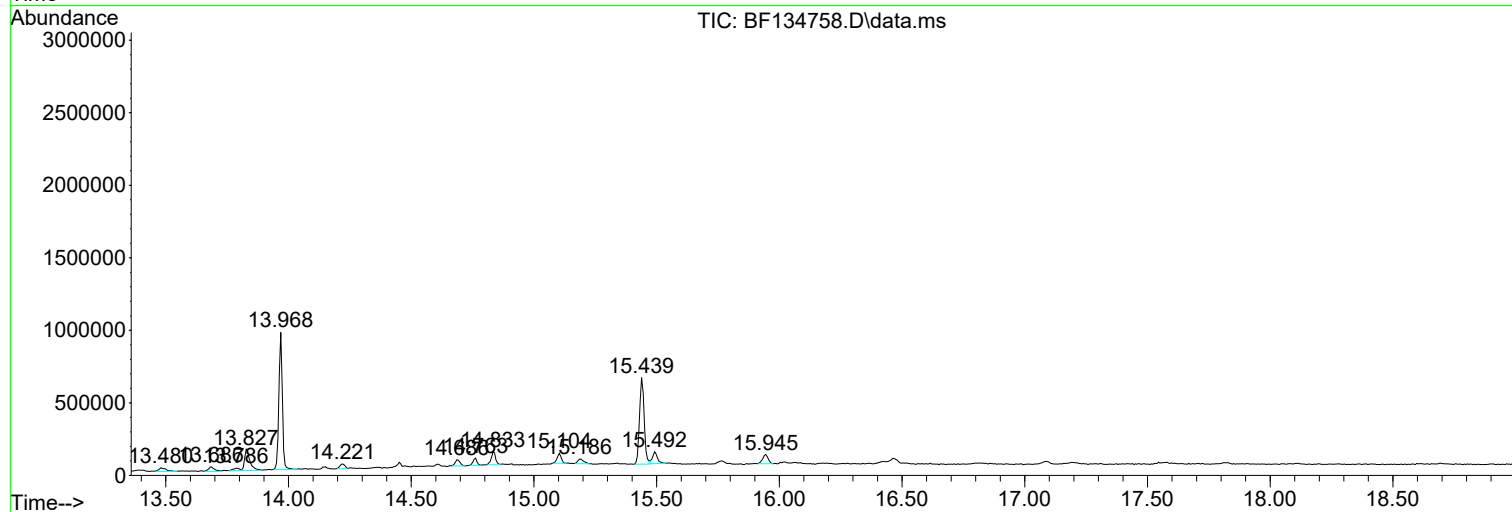
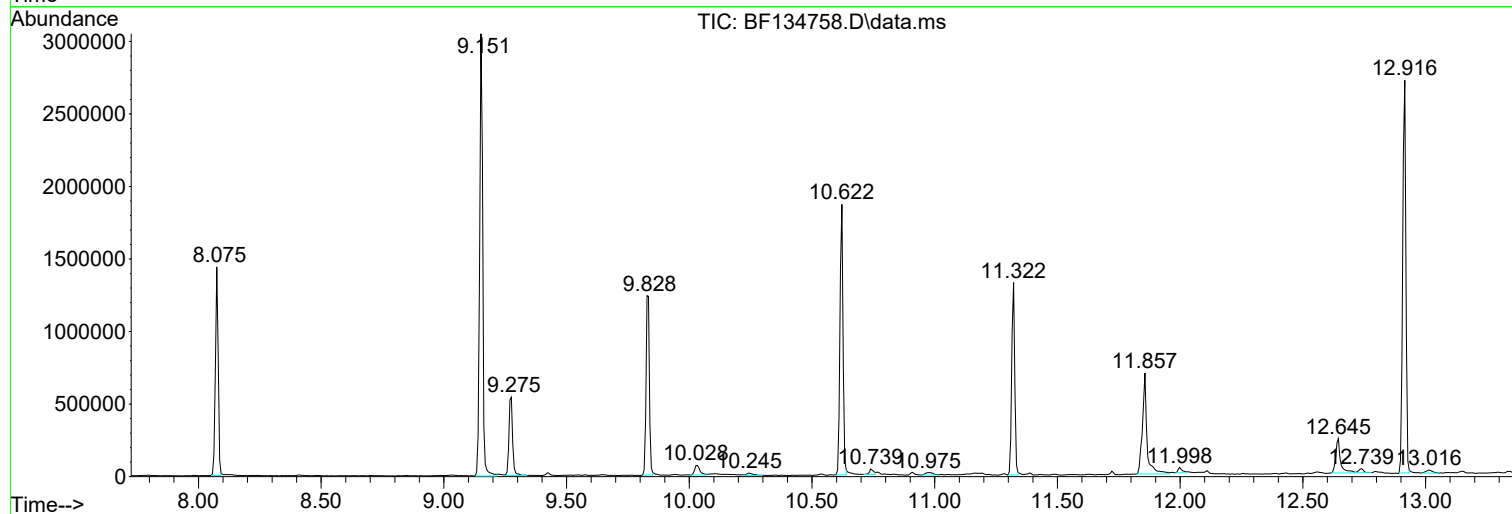
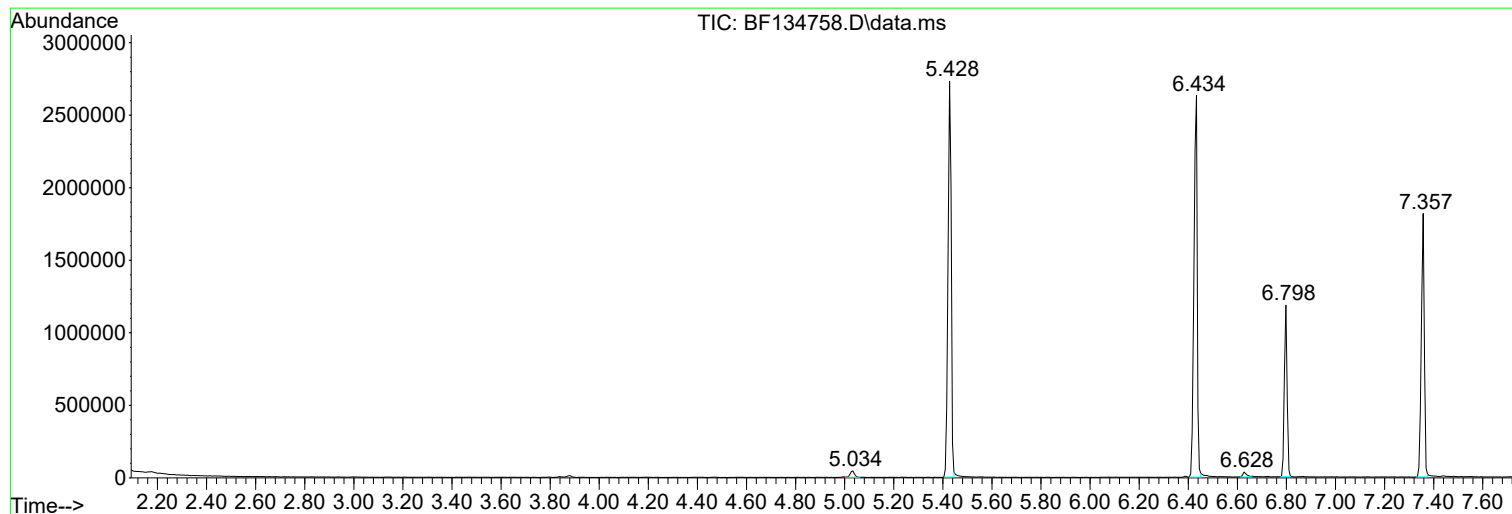
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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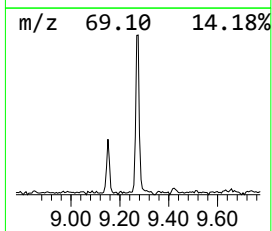
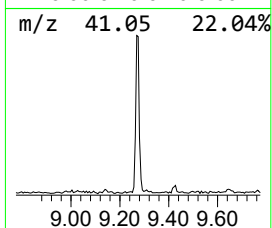
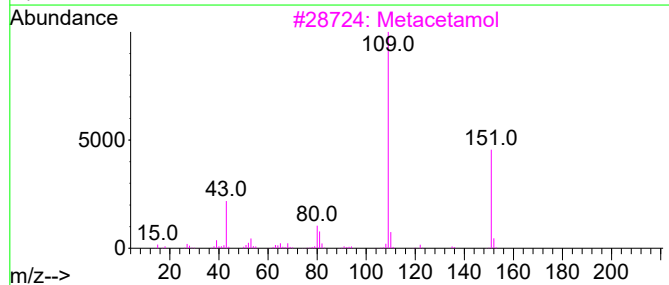
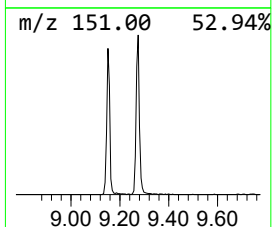
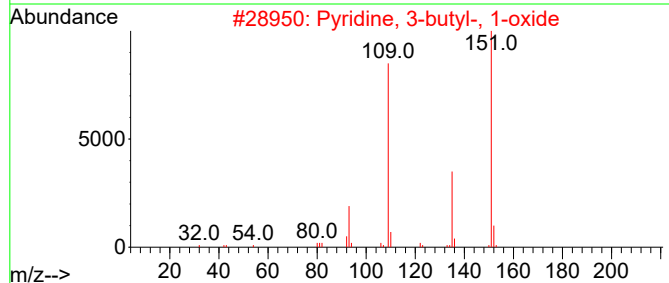
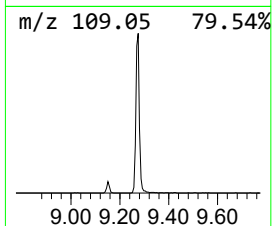
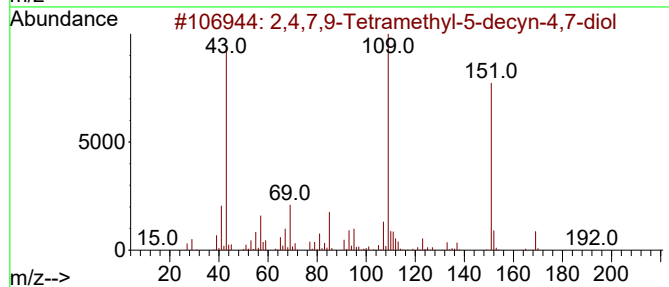
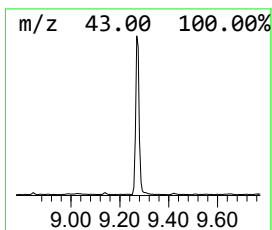
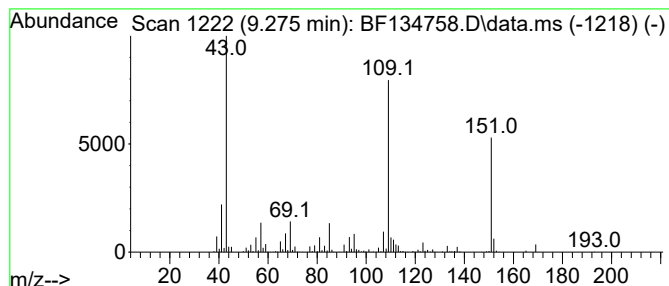
Instrument :
BNA_F
ClientSampleId :
B-PP24B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.275	9.65 ng	562116	Acenaphthene-d10		9.833	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	91
2	Pyridine, 3-butyl-, 1-oxide		151	C9H13NO	031396-33-5	59
3	Metacetamol		151	C8H9NO2	000621-42-1	59
4	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	59
5	1-(1,2,3-Trimethyl-cyclopent-2-e...		152	C10H16O	070987-81-4	43



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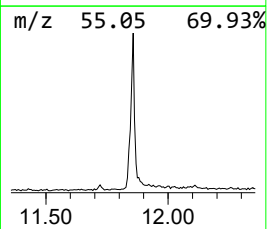
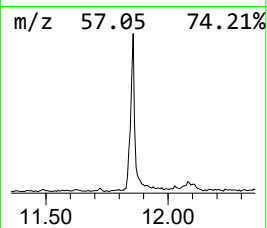
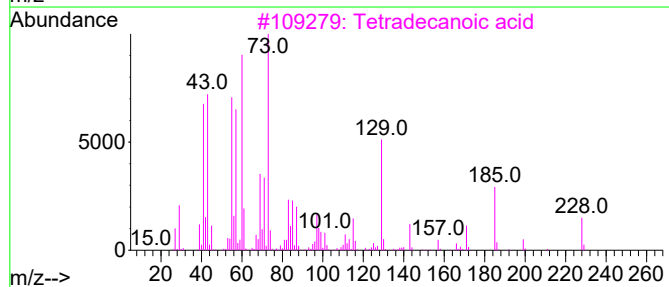
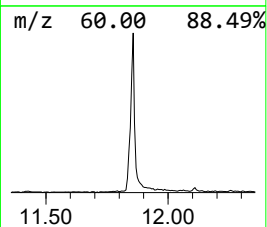
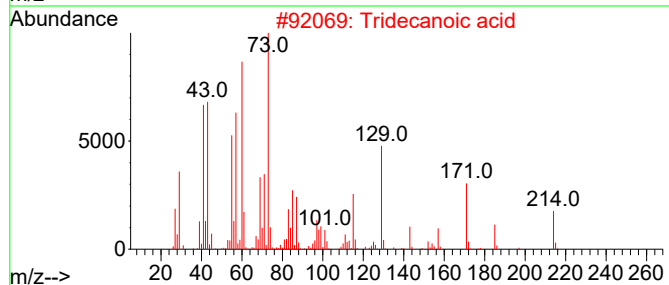
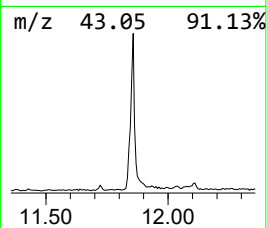
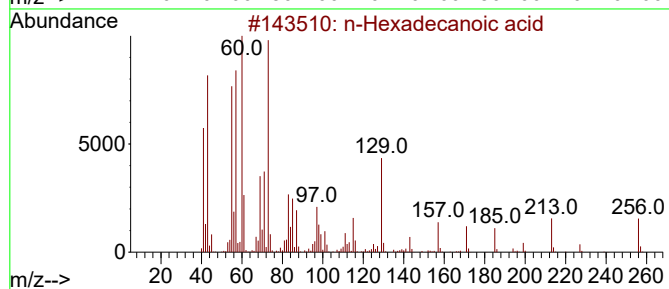
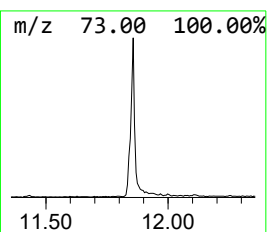
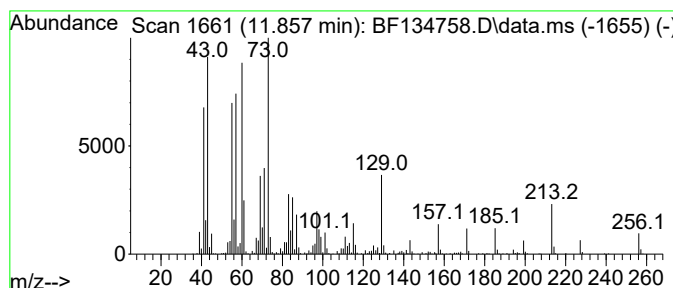
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.857	15.69 ng	892997	Phenanthrene-d10	11.322	
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	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



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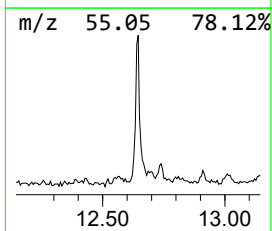
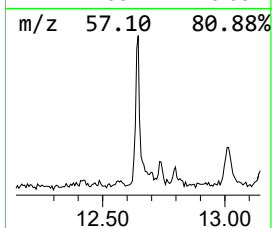
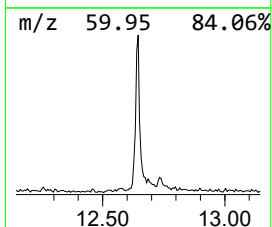
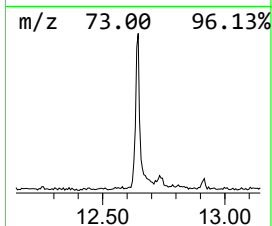
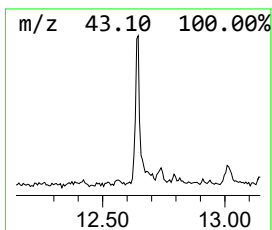
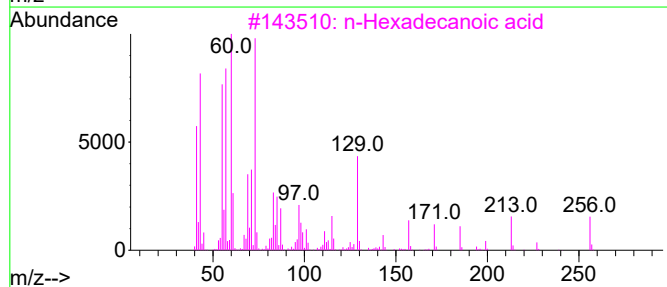
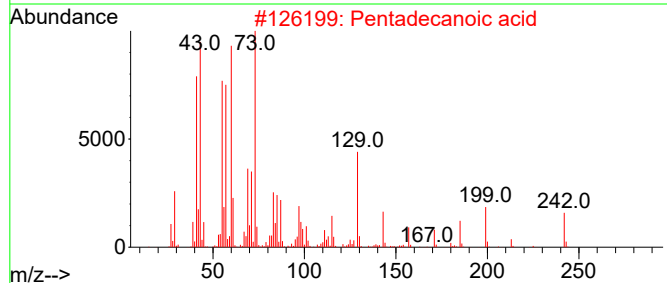
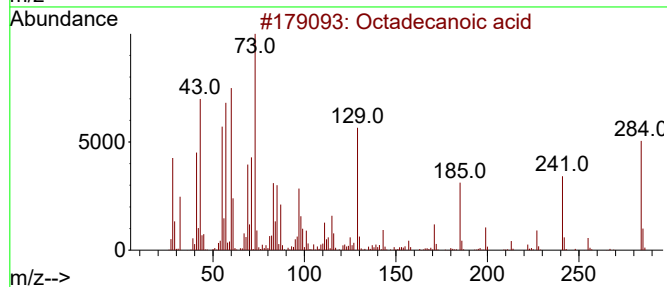
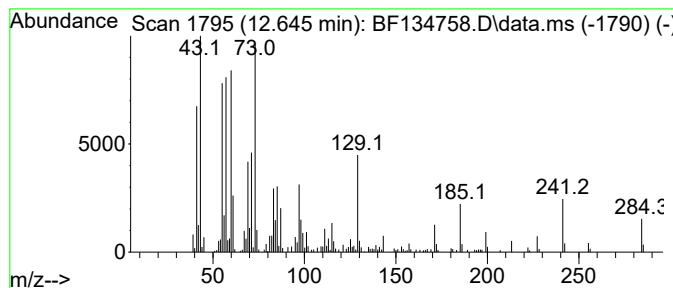
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	5.60 ng	319069	Phenanthrene-d10	11.322

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	93
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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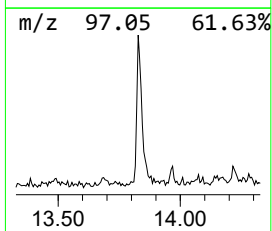
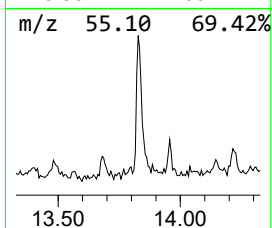
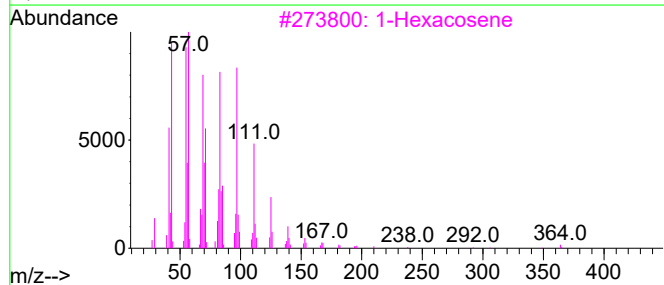
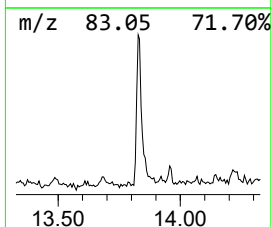
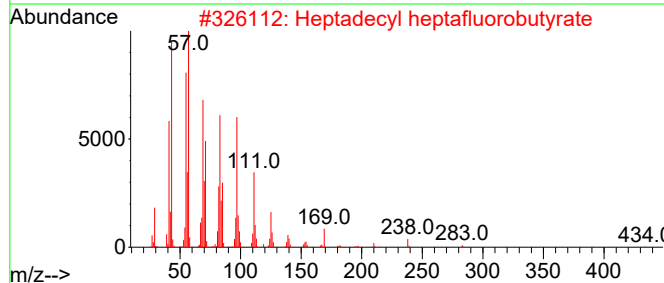
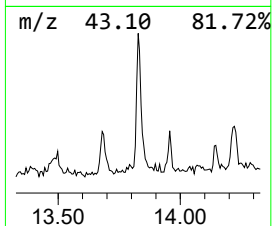
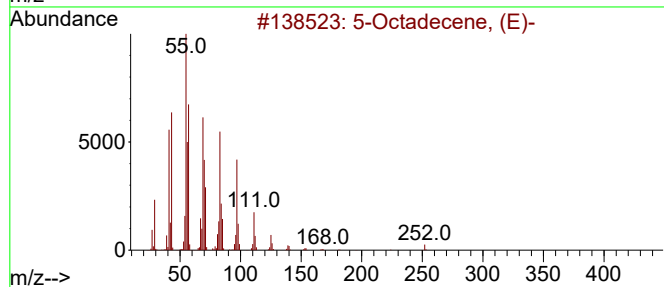
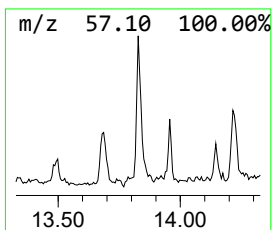
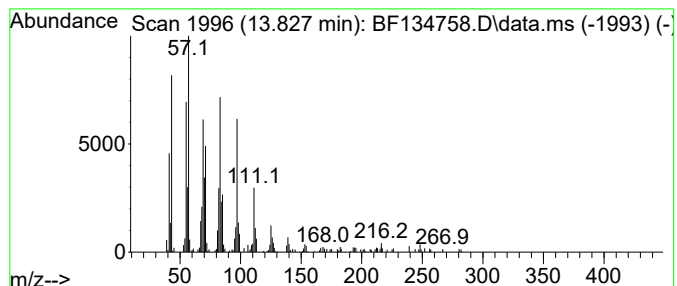
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.68 ng	219372	Chrysene-d12	13.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95	
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94	
3	1-Hexacosene	364	C26H52	018835-33-1	94	
4	1-Octadecene	252	C18H36	000112-88-9	92	
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91	



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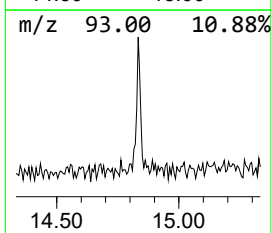
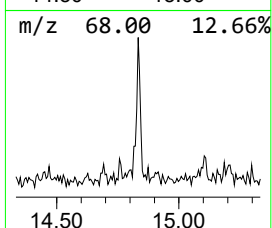
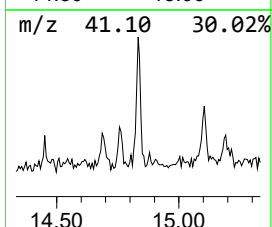
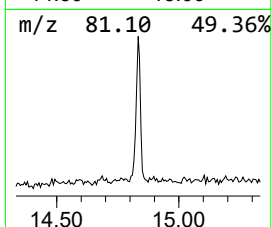
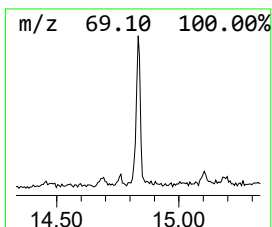
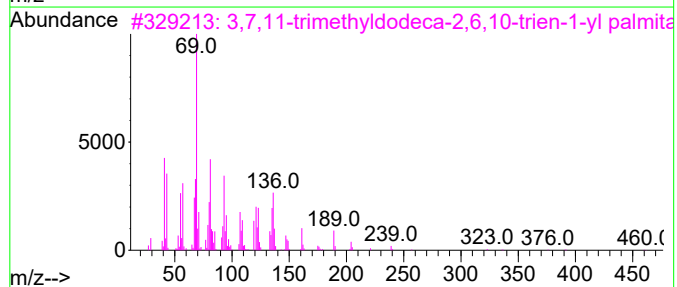
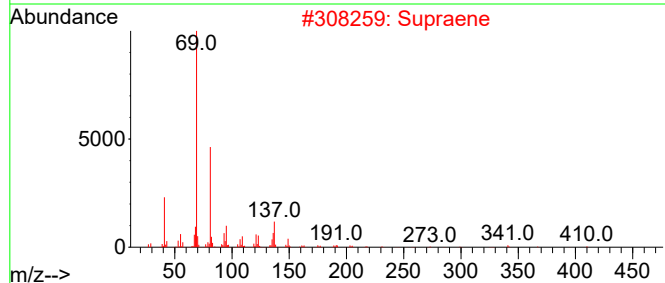
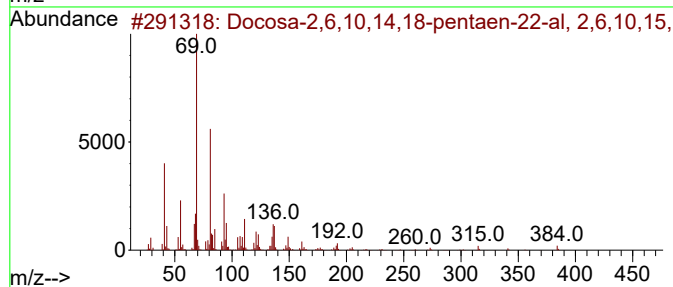
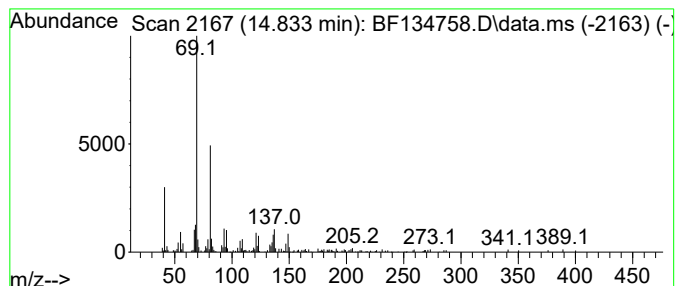
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Docosa-2,6,10,14,18-pentaen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.84 ng	109320	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
2			Supraene	410	C30H50	007683-64-9	74
3			3,7,11-trimethyldodeca-2,6,10-tr...	460	C31H56O2	157501-12-7	64
4			Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	64
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081423\
Data File : BF134758.D
Acq On : 14 Aug 2023 14:26
Operator : CG\JU
Sample : 03989-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP24B

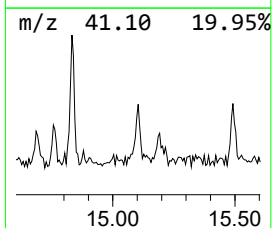
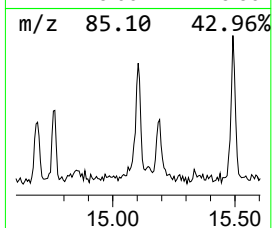
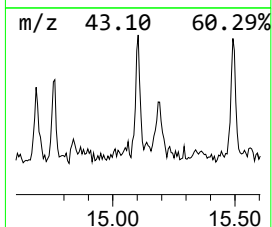
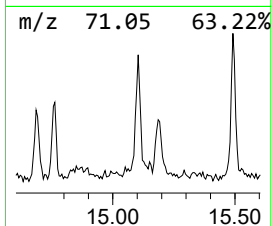
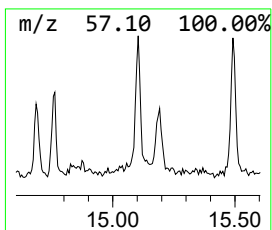
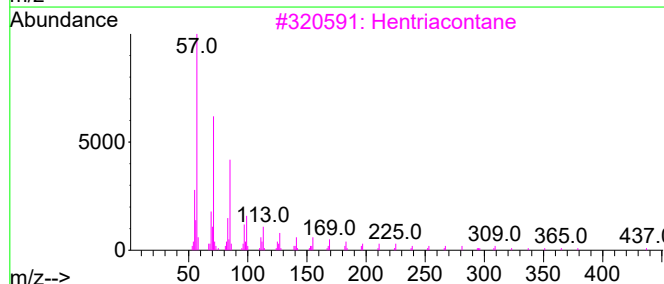
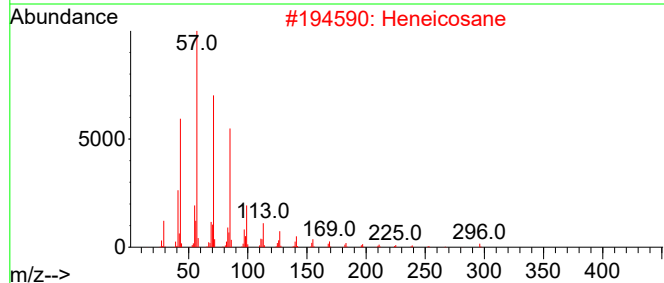
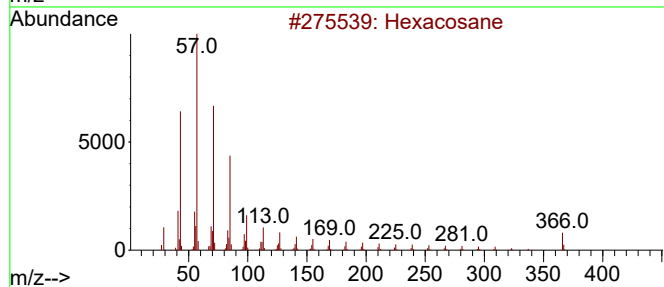
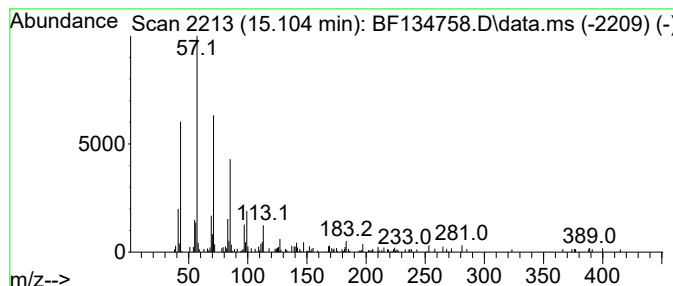
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	2.06 ng	79396	Perylene-d12	15.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	90
2		Heneicosane	296	C21H44	000629-94-7	87
3		Hentriacontane	437	C31H64	000630-04-6	87
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081423\
Data File : BF134758.D
Acq On : 14 Aug 2023 14:26
Operator : CG\JU
Sample : 03989-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP24B

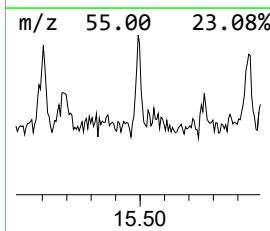
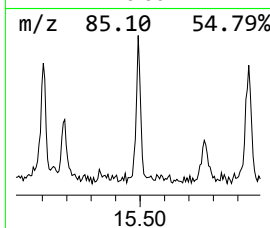
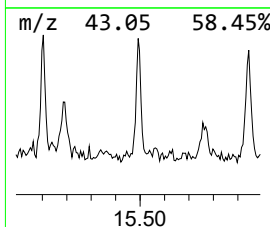
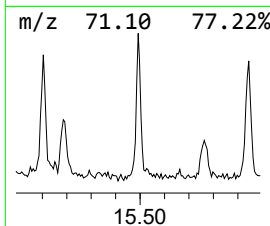
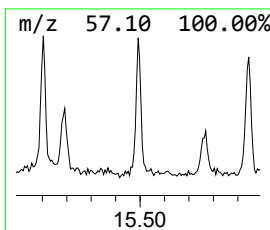
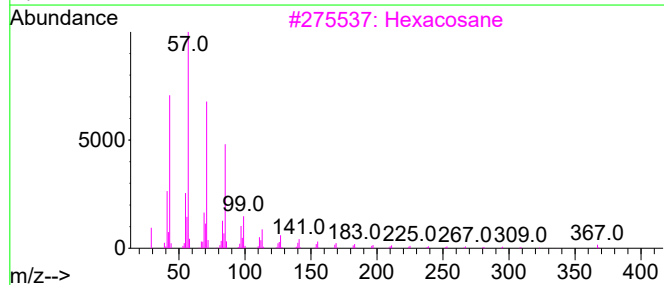
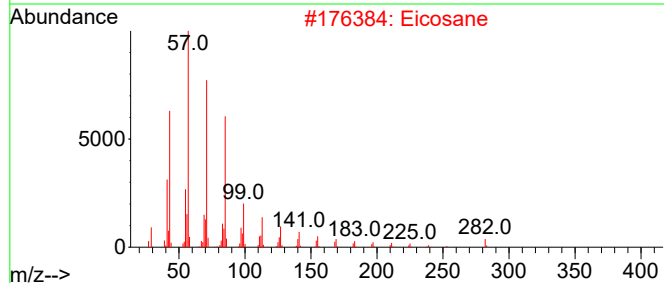
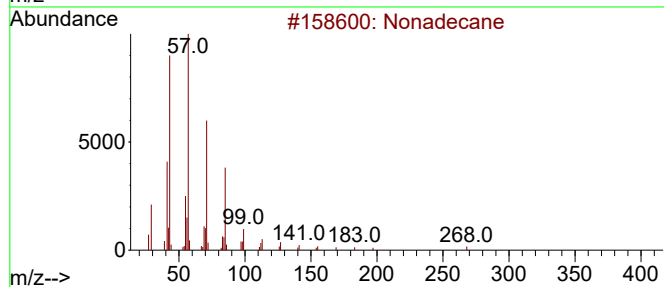
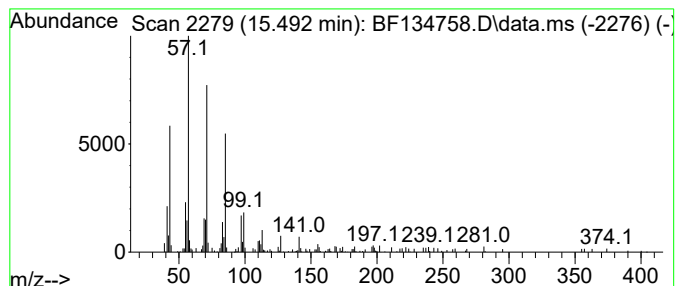
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.492	2.78 ng	107261	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	95
2			Eicosane	282	C20H42	000112-95-8	93
3			Hexacosane	366	C26H54	000630-01-3	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081423\
Data File : BF134758.D
Acq On : 14 Aug 2023 14:26
Operator : CG\JU
Sample : 03989-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP24B

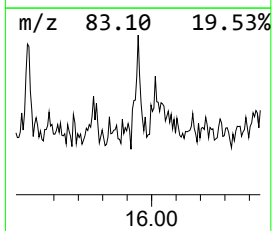
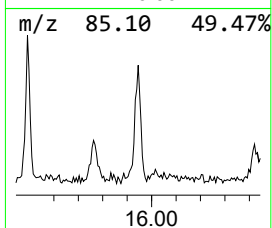
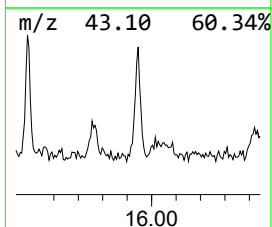
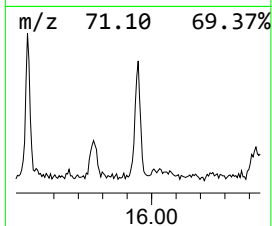
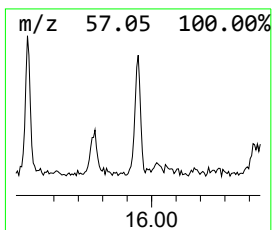
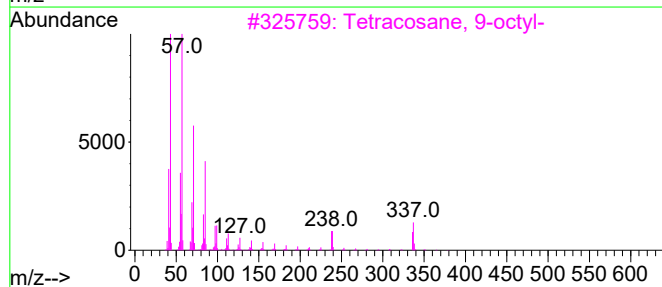
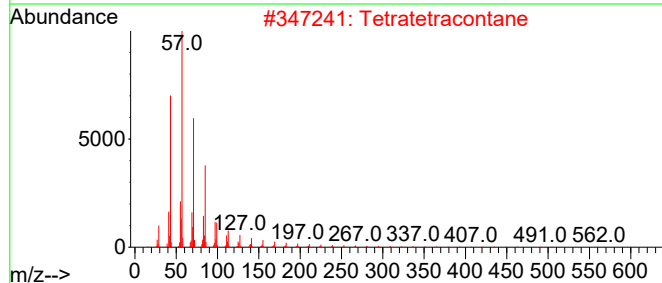
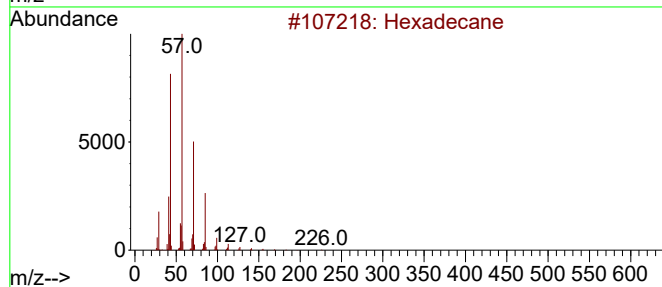
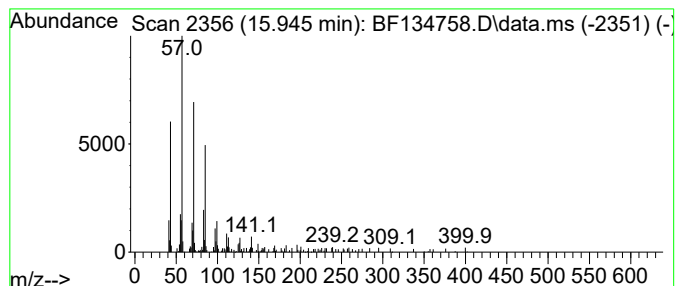
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.49 ng	95880	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	95
2			Tetratetracontane	619	C44H90	007098-22-8	87
3			Tetracosane, 9-octyl-	451	C32H66	055401-54-2	86
4			Octacosane	394	C28H58	000630-02-4	83
5			Hexacosane	366	C26H54	000630-01-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081423\
Data File : BF134758.D
Acq On : 14 Aug 2023 14:26
Operator : CG\JU
Sample : 03989-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP24B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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
2,4,7,9-Tetrame...	9.275	9.7	ng	562116	3	9.833	1165200	20.0
n-Hexadecanoic ...	11.857	15.7	ng	892997	4	11.322	1138600	20.0
Octadecanoic acid	12.645	5.6	ng	319069	4	11.322	1138600	20.0
5-Octadecene, (E)-	13.827	4.7	ng	219372	5	13.969	936949	20.0
Docosa-2,6,10,1...	14.833	2.8	ng	109320	6	15.439	771059	20.0
Hexacosane	15.104	2.1	ng	79396	6	15.439	771059	20.0
Nonadecane	15.492	2.8	ng	107261	6	15.439	771059	20.0
Hexadecane	15.945	2.5	ng	95880	6	15.439	771059	20.0