

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
 Data File : BF133080.D
 Acq On : 26 Apr 2023 23:04
 Operator : CG\JU
 Sample : 02270-20
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-30-0-2-20230412

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133080.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.916	477	481	492	rVB	141081	174253	4.87%	0.625%
2	5.340	548	553	556	rBV	3162671	2921410	81.72%	10.475%
3	6.275	709	712	716	rBV	277765	214476	6.00%	0.769%
4	6.369	723	728	731	rBV	3267425	2921984	81.74%	10.477%
5	6.734	786	790	793	rBV	1264657	984618	27.54%	3.530%
6	7.298	881	886	889	rBV	2191250	1967983	55.05%	7.056%
7	8.016	1004	1008	1011	rBV	1732625	1347873	37.70%	4.833%
8	8.745	1126	1132	1144	rBV2	32075	44983	1.26%	0.161%
9	9.092	1187	1191	1194	rBV	4416543	3574909	100.00%	12.818%
10	9.769	1302	1306	1309	rBV	2009372	1518622	42.48%	5.445%
11	10.480	1423	1427	1430	rBV	172558	131897	3.69%	0.473%
12	10.557	1435	1440	1443	rBV	2248944	2110200	59.03%	7.566%
13	11.251	1554	1558	1560	rBV	1845112	1563015	43.72%	5.604%
14	11.269	1560	1561	1564	rVB	91103	66338	1.86%	0.238%
15	11.557	1607	1610	1613	rBV	69037	58252	1.63%	0.209%
16	11.786	1645	1649	1653	rBV2	416467	374479	10.48%	1.343%
17	12.357	1739	1746	1751	rBV5	40551	69032	1.93%	0.248%
18	12.457	1759	1763	1767	rBV	180010	147782	4.13%	0.530%
19	12.551	1777	1779	1781	rBV	62004	58700	1.64%	0.210%
20	12.569	1781	1782	1794	rVB4	67949	87952	2.46%	0.315%
21	12.657	1794	1797	1799	rBV2	124894	133949	3.75%	0.480%
22	12.680	1799	1801	1805	rVB	217622	214437	6.00%	0.769%
23	12.839	1823	1828	1831	rBV	3913411	3496830	97.82%	12.538%
24	13.798	1985	1991	1993	rBV2	63657	115169	3.22%	0.413%
25	13.880	2001	2005	2008	rBV	1262026	1191049	33.32%	4.271%
26	13.904	2008	2009	2015	rVB	83573	73069	2.04%	0.262%
27	14.374	2085	2089	2092	rBV	68410	67686	1.89%	0.243%
28	14.804	2159	2162	2171	rVB	175250	198281	5.55%	0.711%
29	14.898	2174	2178	2181	rBV	54134	78798	2.20%	0.283%
30	14.992	2190	2194	2201	rVB	151768	167472	4.68%	0.600%
31	15.180	2223	2226	2231	rVB	48374	66418	1.86%	0.238%
32	15.239	2233	2236	2241	rVB	52067	61357	1.72%	0.220%
33	15.304	2242	2247	2253	rVV	867933	1060900	29.68%	3.804%
34	15.351	2253	2255	2261	rVB3	38105	51552	1.44%	0.185%
35	15.545	2284	2288	2294	rVB	52279	68924	1.93%	0.247%
36	15.768	2321	2326	2332	rBV	139579	197592	5.53%	0.708%

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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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.515	2448	2453	2462	rVB4	70905	127684	3.57%	0.458%
38	16.804	2497	2502	2508	rBV2	54716	109523	3.06%	0.393%
39	17.015	2535	2538	2544	rVB5	41774	69966	1.96%	0.251%

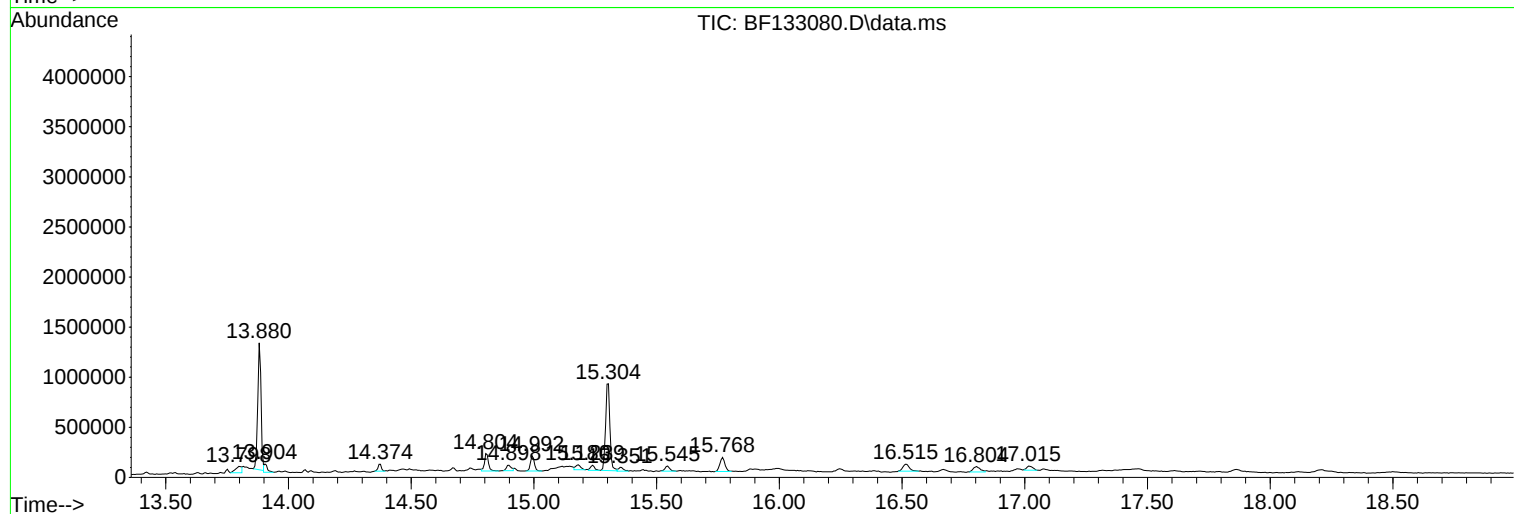
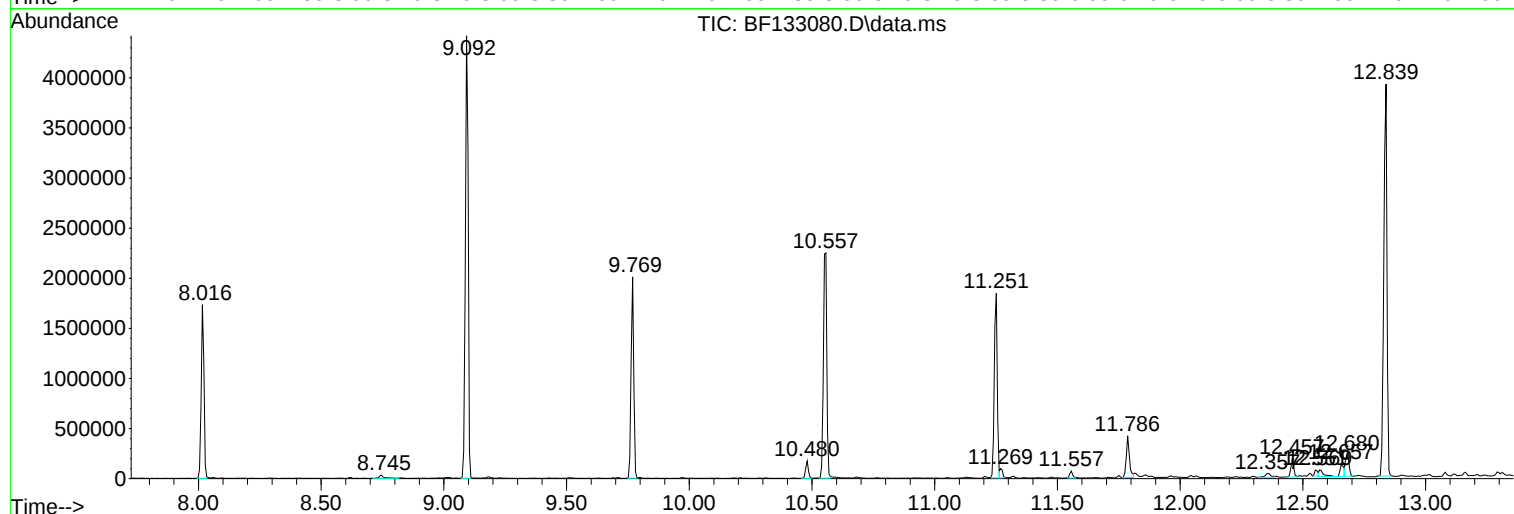
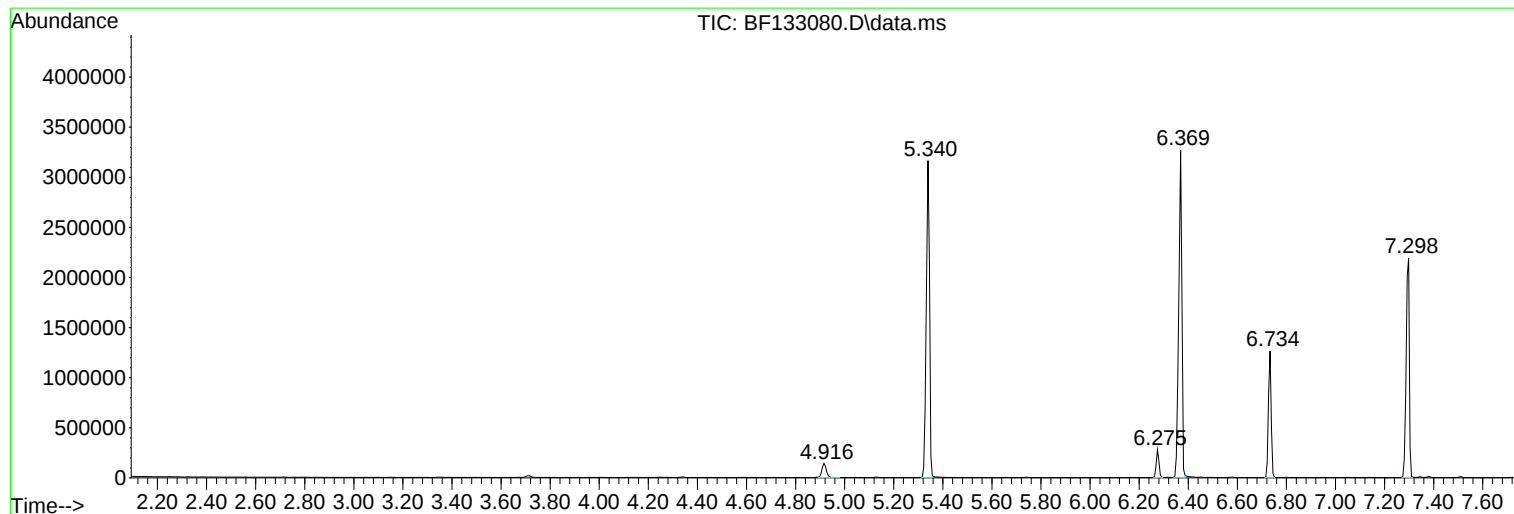
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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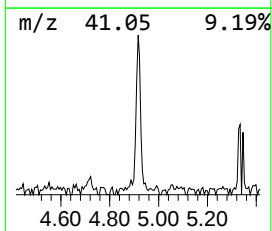
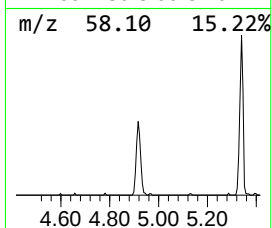
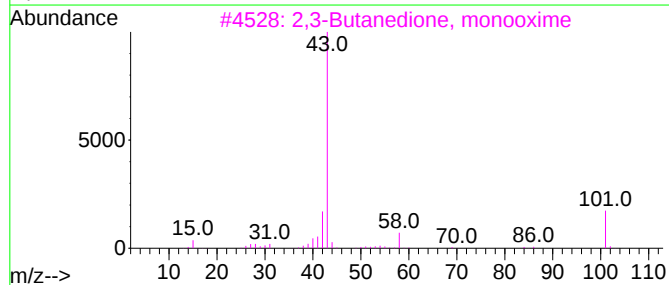
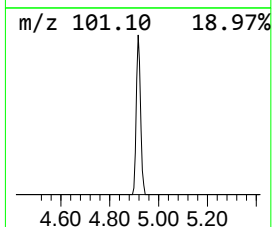
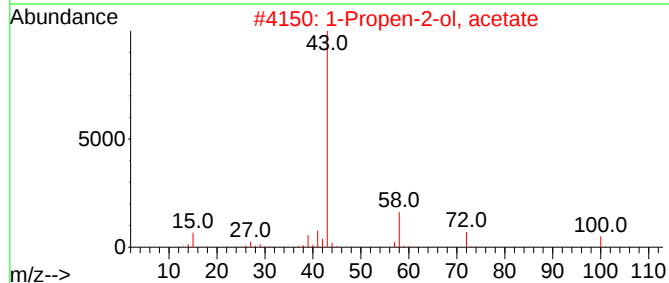
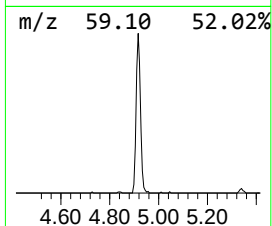
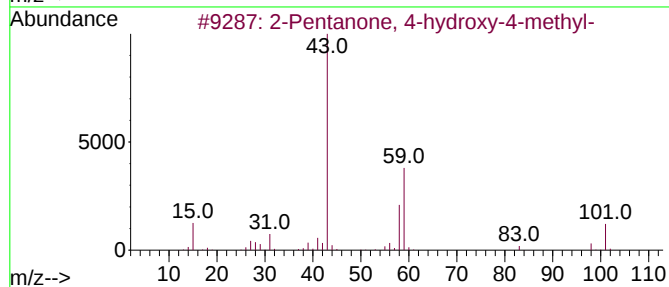
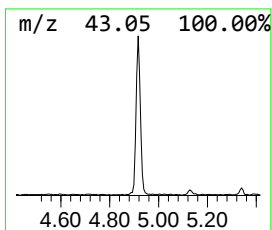
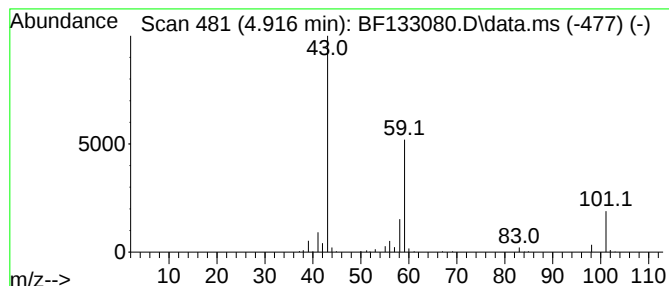
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.916	3.54 ng	174253	1,4-Dichlorobenzene-d4	6.734

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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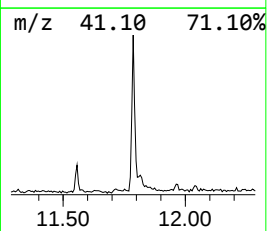
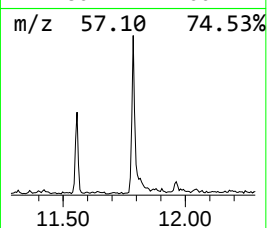
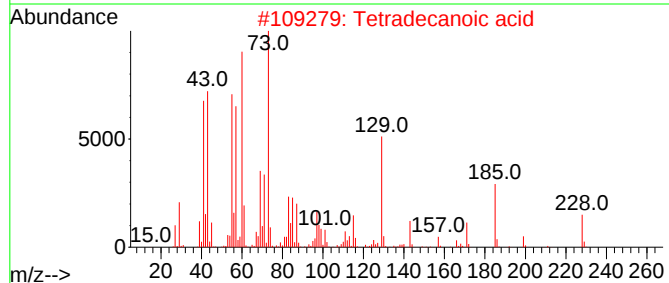
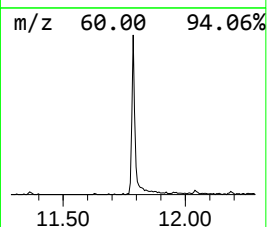
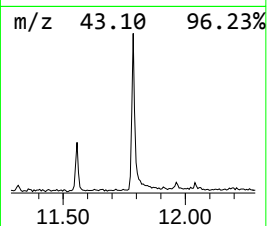
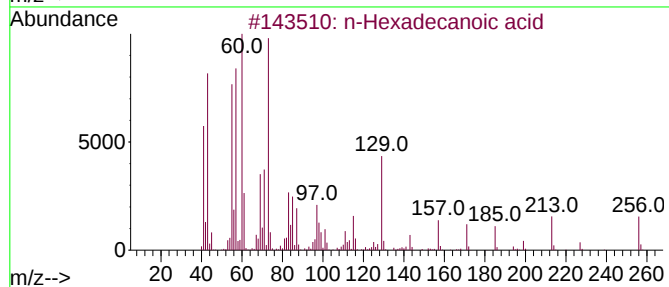
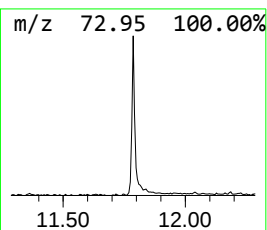
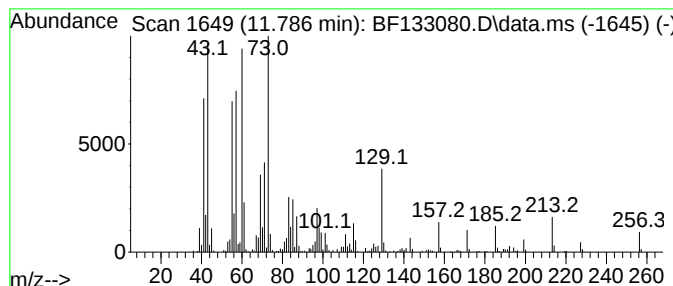
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	4.79 ng	374479	Phenanthrene-d10	11.251

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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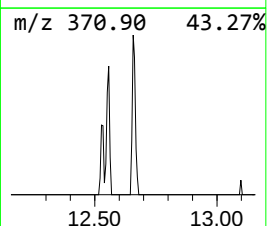
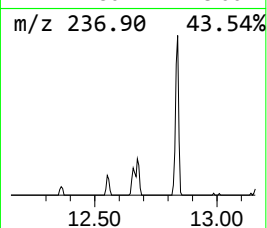
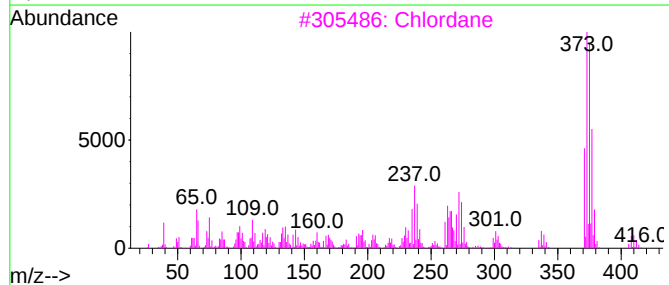
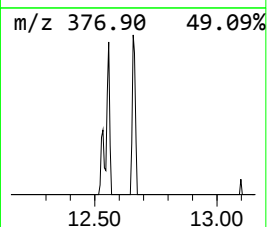
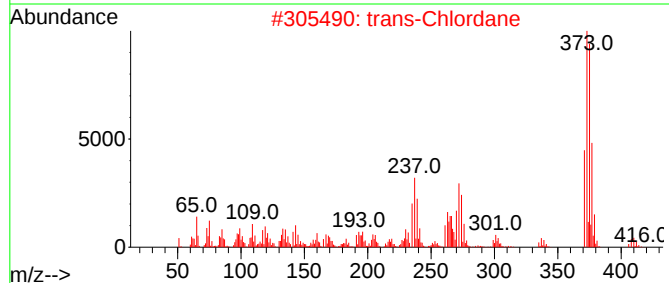
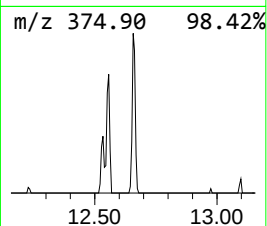
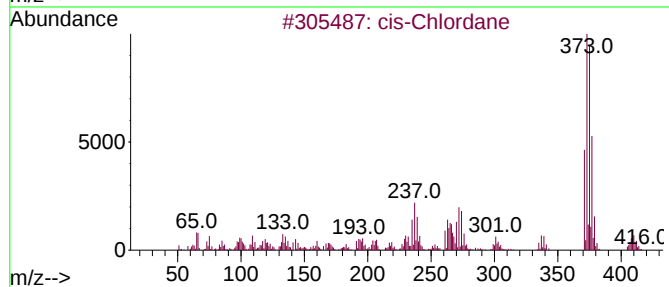
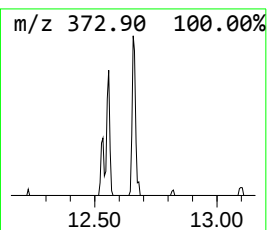
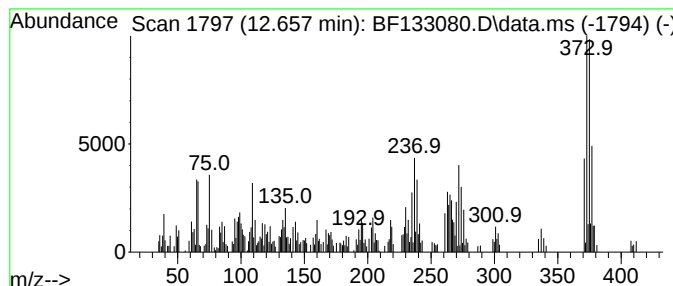
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 cis-Chlordane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	2.25 ng	133949	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Chlordane	406	C10H6Cl8	005103-71-9	99
2			trans-Chlordane	406	C10H6Cl8	005103-74-2	99
3			Chlordane	406	C10H6Cl8	000057-74-9	99
4			Monomethyltetrachloroterephthala...	388	C12H12Cl4O4Si	1000485-37-8	35
5			4,7-Methanoindene, 1,2,3,5,6,7,8...	406	C10H6Cl8	1000017-10-9	35



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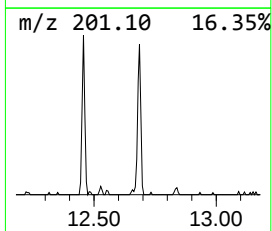
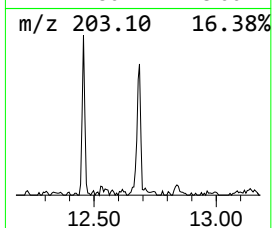
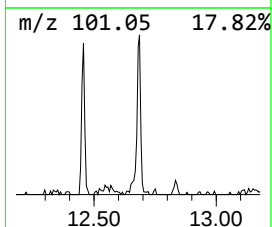
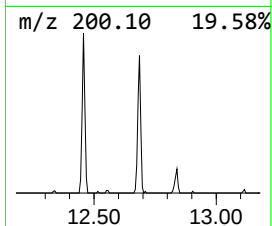
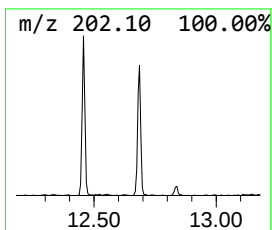
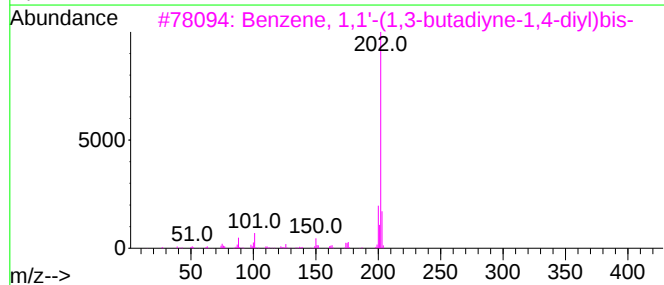
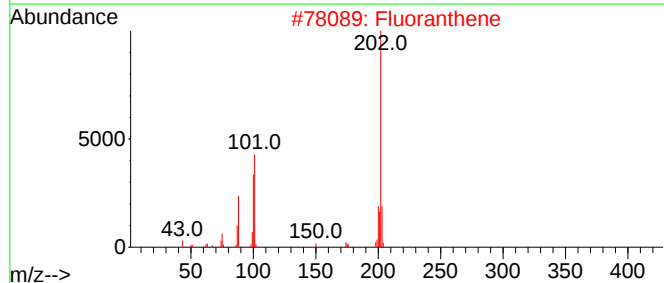
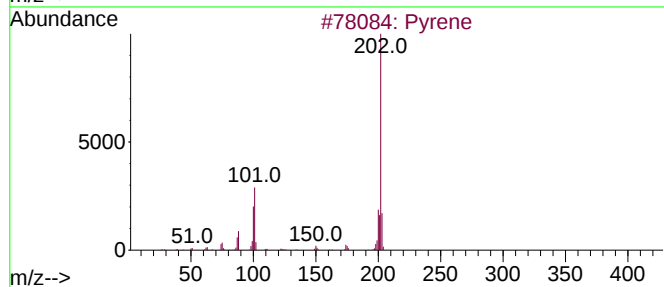
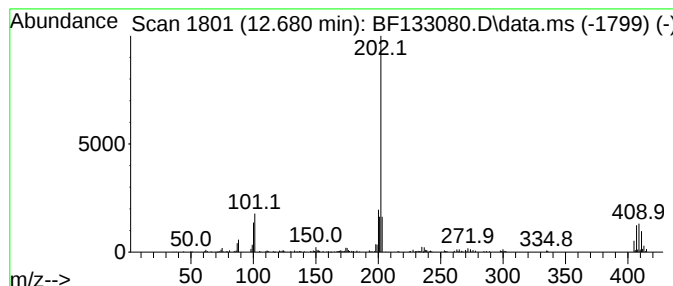
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown12.680 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	3.60 ng	214437	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	90
2			Fluoranthene	202	C16H10	000206-44-0	55
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	43
4			4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	37
5			l-Leucine, N-methyl-N-(2-methoxy...	331	C17H33NO5	1000328-54-1	37



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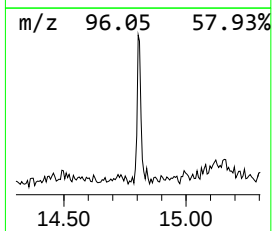
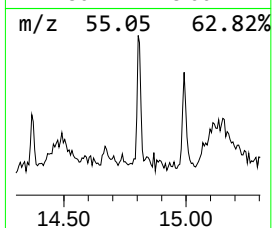
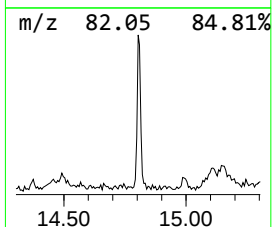
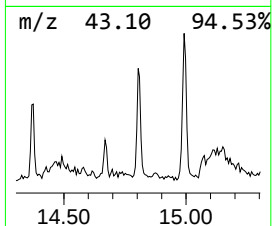
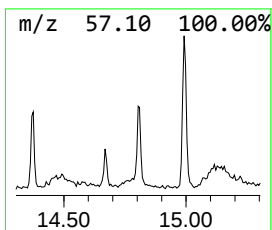
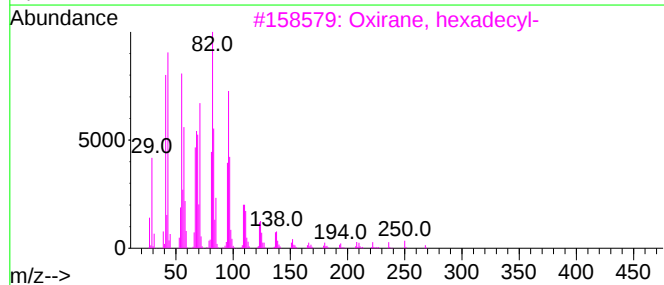
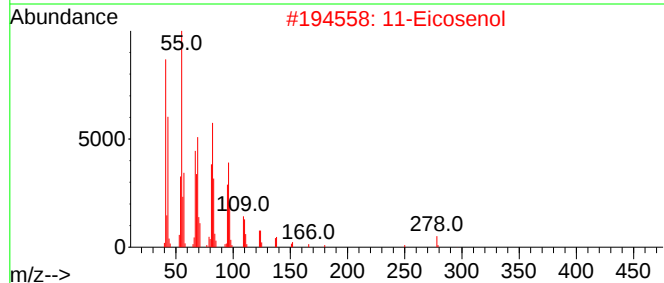
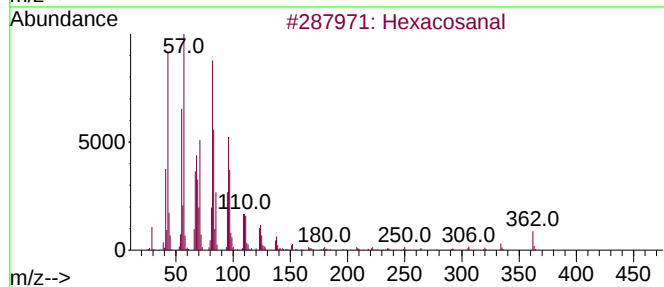
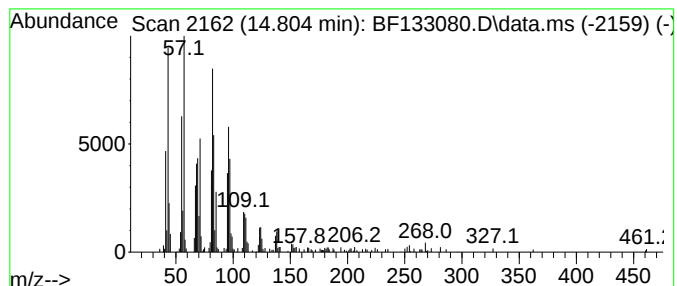
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	3.74 ng	198281	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosanal	380	C26H52O	026627-85-0	94
2			11-Eicosenol	296	C20H40O	1010424-20-3	93
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5			Eicosanal-	296	C20H40O	002400-66-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133080.D
Acq On : 26 Apr 2023 23:04
Operator : CG\JU
Sample : 02270-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-30-0-2-20230412

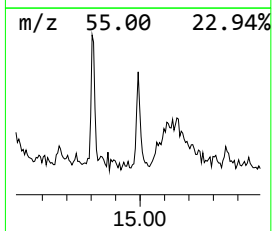
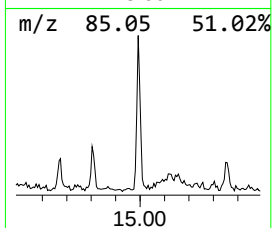
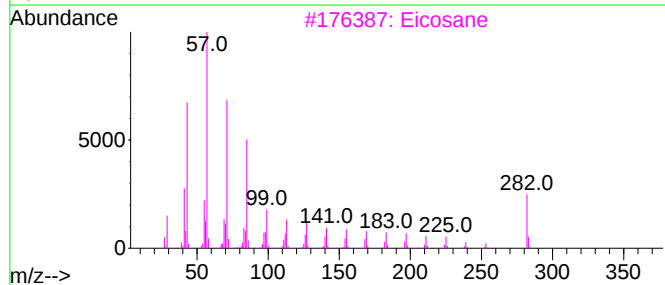
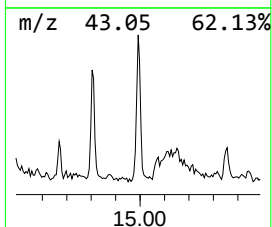
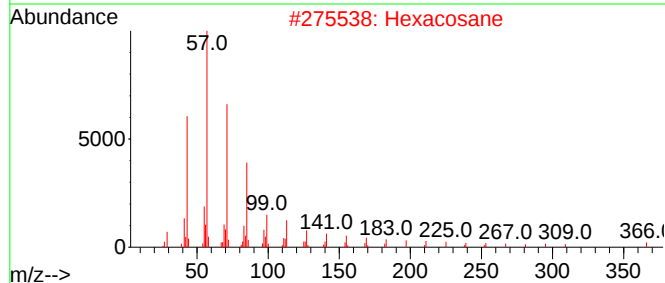
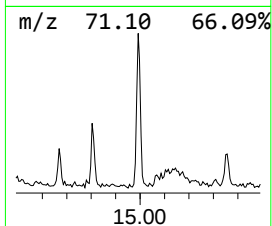
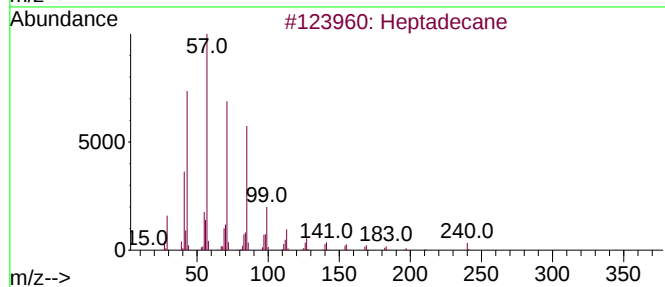
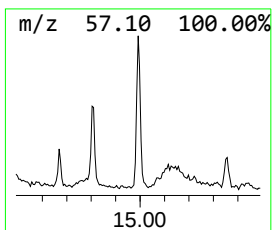
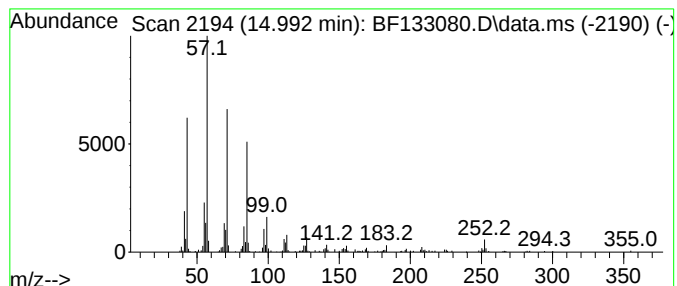
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	3.16 ng	167472	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	83
2			Hexacosane	366	C26H54	000630-01-3	83
3			Eicosane	282	C20H42	000112-95-8	81
4			Octacosane	394	C28H58	000630-02-4	76
5			Tetratetracontane	619	C44H90	007098-22-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133080.D
Acq On : 26 Apr 2023 23:04
Operator : CG\JU
Sample : 02270-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-30-0-2-20230412

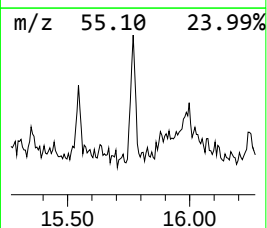
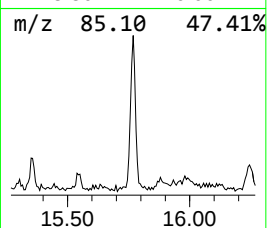
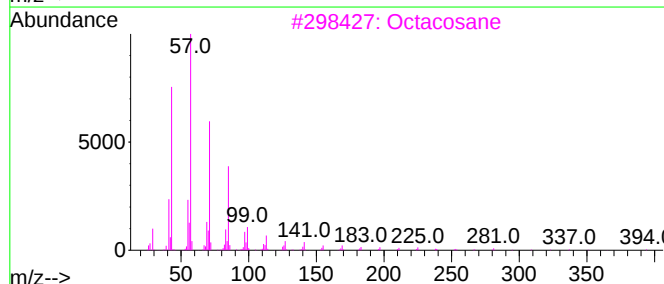
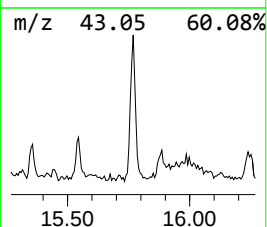
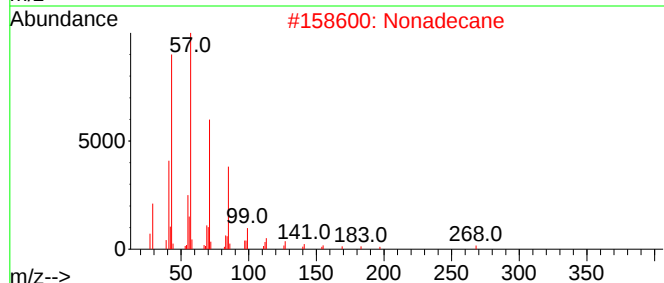
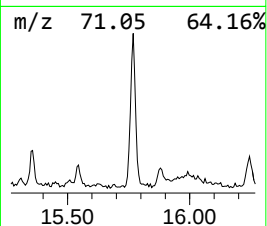
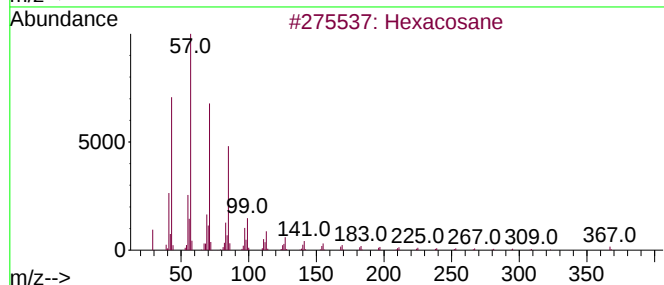
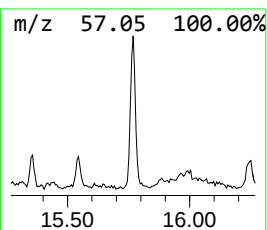
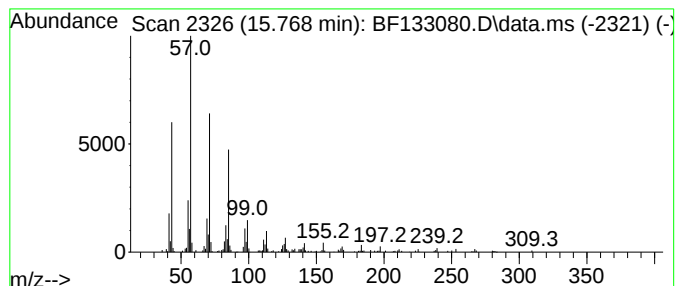
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.768	3.72 ng	197592	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Nonadecane	268	C19H40	000629-92-5	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133080.D
Acq On : 26 Apr 2023 23:04
Operator : CG\JU
Sample : 02270-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-30-0-2-20230412

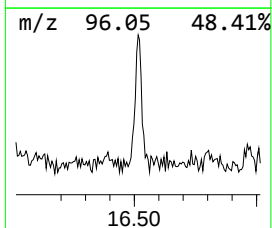
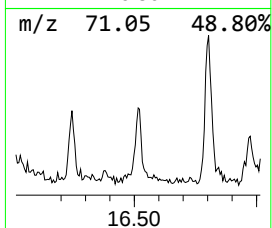
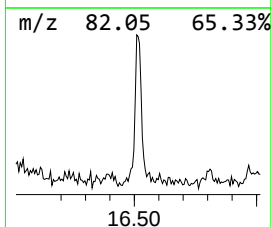
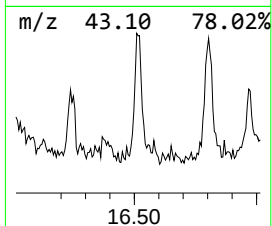
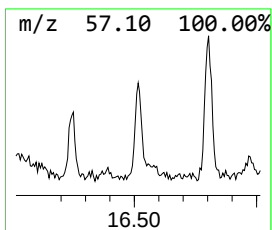
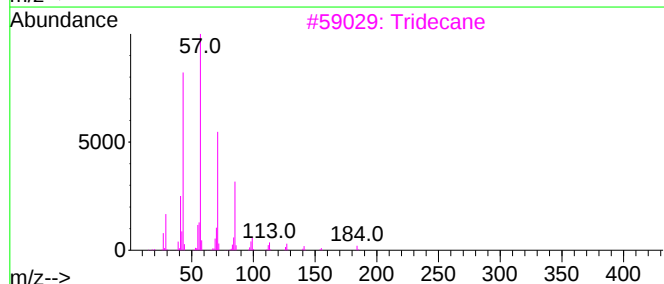
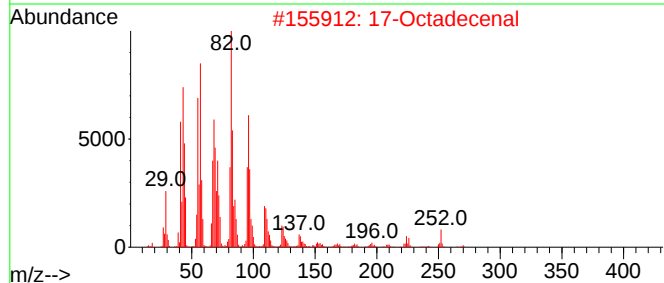
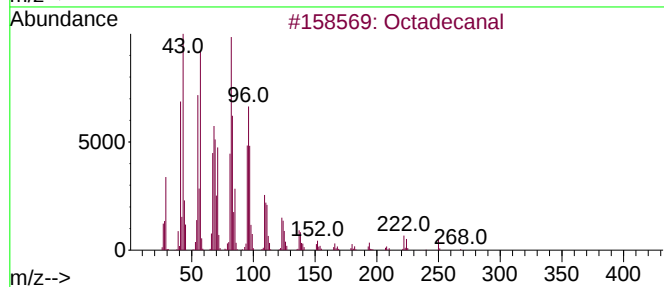
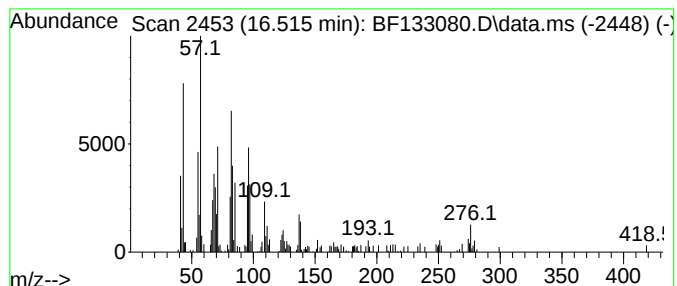
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.515	2.41 ng	127684	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	72
2			17-Octadecenal	266	C18H34O	056554-86-0	72
3			Tridecane	184	C13H28	000629-50-5	56
4			1,7-Hexadecadiene	222	C16H30	125110-62-5	43
5			2-Heptadecenal	252	C17H32O	1000143-48-6	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133080.D
Acq On : 26 Apr 2023 23:04
Operator : CG\JU
Sample : 02270-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-30-0-2-20230412

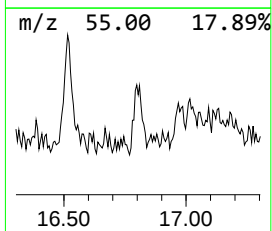
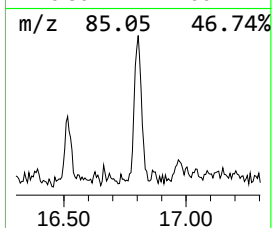
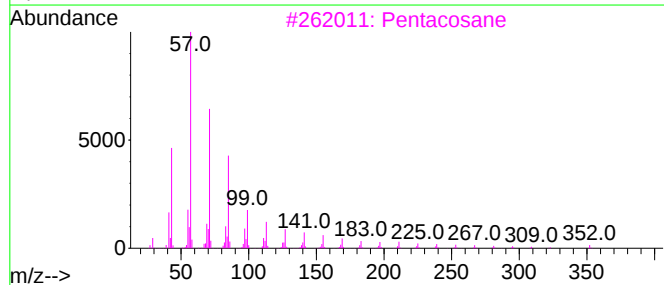
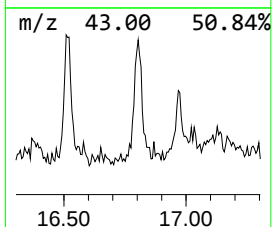
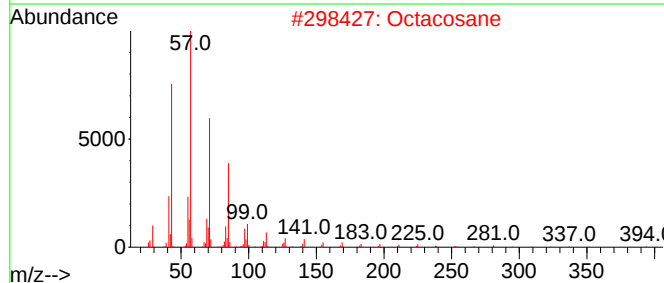
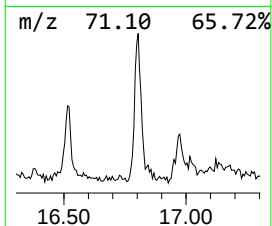
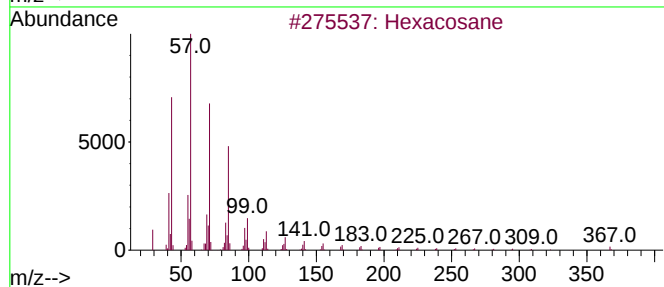
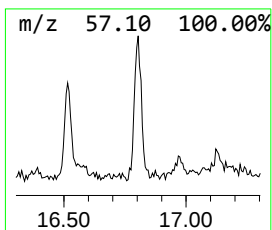
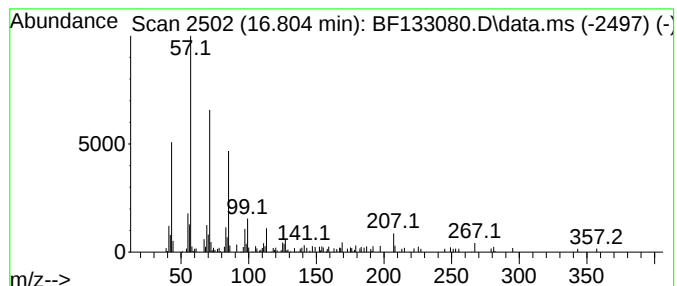
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.804	2.06 ng	109523	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Tetracosane	338	C24H50	000646-31-1	86
5		triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133080.D
Acq On : 26 Apr 2023 23:04
Operator : CG\JU
Sample : 02270-20
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-30-0-2-20230412

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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n-Hexadecanoic ...	11.786	4.8	ng	374479	4	11.251	1563020	20.0
cis-Chlordane	12.657	2.3	ng	133949	5	13.880	1191050	20.0
unknown12.680	12.680	3.6	ng	214437	5	13.880	1191050	20.0
Hexacosanal	14.804	3.7	ng	198281	6	15.304	1060900	20.0
Heptadecane	14.992	3.2	ng	167472	6	15.304	1060900	20.0
Hexacosane	15.768	3.7	ng	197592	6	15.304	1060900	20.0
Octadecanal	16.515	2.4	ng	127684	6	15.304	1060900	20.0
Octacosane	16.804	2.1	ng	109523	6	15.304	1060900	20.0