

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
 Data File : BF136740.D
 Acq On : 27 Dec 2023 02:12
 Operator : CG\JU
 Sample : 05602-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPRING-VALLEY-TP-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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136740.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	9	15	24	rVB2	19127	30668	2.14%	0.292%
2	5.022	495	499	505	rVB	66076	77754	5.42%	0.741%
3	5.428	564	568	579	rBV	1495921	1315428	91.73%	12.532%
4	6.428	734	738	741	rBV	1304924	1278790	89.17%	12.183%
5	6.781	795	798	802	rBV	504641	411370	28.69%	3.919%
6	7.345	889	894	897	rBV	978915	841607	58.69%	8.018%
7	8.057	1012	1015	1019	rBV	583276	479964	33.47%	4.572%
8	9.139	1194	1199	1202	rBV	1614600	1434032	100.00%	13.662%
9	9.816	1310	1314	1317	rBV	572347	428774	29.90%	4.085%
10	10.610	1445	1449	1452	rBV	720543	616944	43.02%	5.877%
11	11.169	1540	1544	1548	rBV	30790	30464	2.12%	0.290%
12	11.257	1557	1559	1564	rVB3	19524	18837	1.31%	0.179%
13	11.310	1564	1568	1570	rBV	439490	411424	28.69%	3.920%
14	11.327	1570	1571	1575	rVB	65678	50711	3.54%	0.483%
15	11.774	1642	1647	1650	rBV3	17650	25293	1.76%	0.241%
16	11.810	1650	1653	1655	rVV2	21665	19088	1.33%	0.182%
17	11.839	1655	1658	1665	rVV	161581	166153	11.59%	1.583%
18	12.022	1682	1689	1691	rBV8	18597	23901	1.67%	0.228%
19	12.404	1749	1754	1758	rBV7	15137	20891	1.46%	0.199%
20	12.527	1771	1775	1778	rBV	130704	122478	8.54%	1.167%
21	12.569	1778	1782	1787	rVB7	15310	35157	2.45%	0.335%
22	12.633	1789	1793	1797	rBV2	34124	43323	3.02%	0.413%
23	12.757	1808	1814	1817	rBV	115759	114685	8.00%	1.093%
24	12.821	1823	1825	1829	rVB2	15579	16469	1.15%	0.157%
25	12.904	1835	1839	1842	rBV	1537404	1277682	89.10%	12.172%
26	13.221	1891	1893	1901	rVB8	11194	21356	1.49%	0.203%
27	13.339	1910	1913	1916	rBV2	37319	44100	3.08%	0.420%
28	13.374	1916	1919	1926	rVB4	33693	59849	4.17%	0.570%
29	13.598	1955	1957	1960	rVB	17942	16481	1.15%	0.157%
30	13.810	1991	1993	1996	rBV3	25783	25637	1.79%	0.244%
31	13.857	1996	2001	2004	rBV5	30422	63187	4.41%	0.602%
32	13.963	2014	2019	2022	rBV2	500726	503209	35.09%	4.794%
33	13.986	2022	2023	2027	rVB	69563	45536	3.18%	0.434%
34	15.010	2194	2197	2199	rBV	53669	63626	4.44%	0.606%
35	15.092	2208	2211	2214	rVB	41015	37933	2.65%	0.361%
36	15.374	2257	2259	2266	rVB	41855	56701	3.95%	0.540%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.439	2266	2270	2274	rBV	210881	267332	18.64%	2.547%
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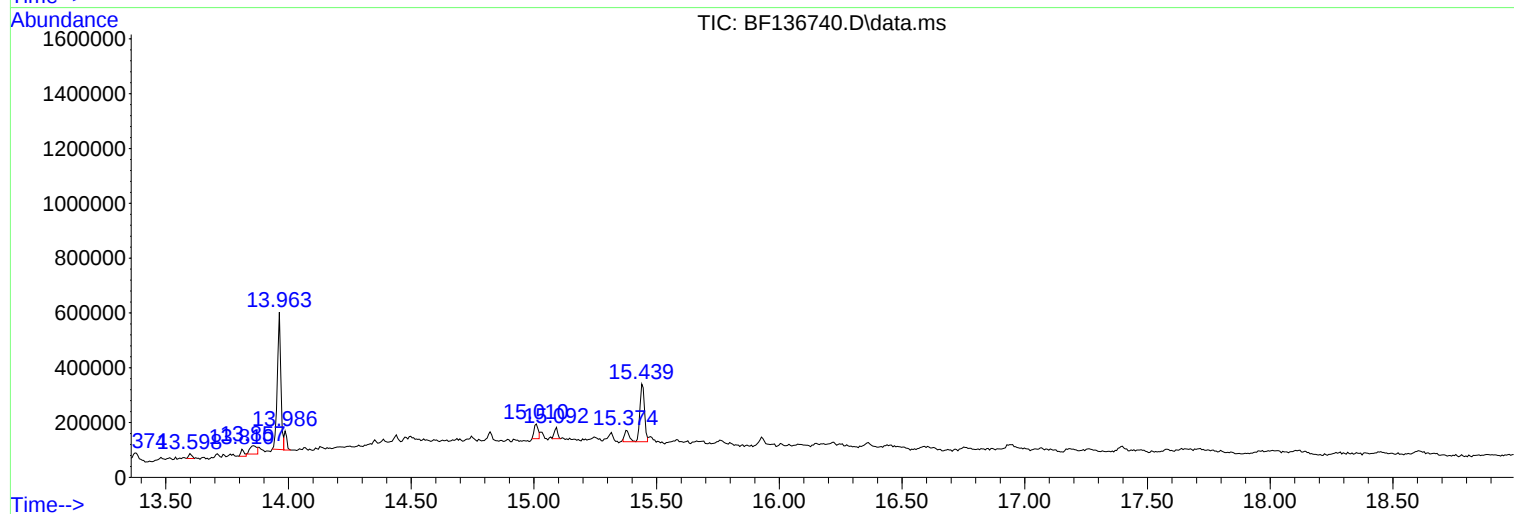
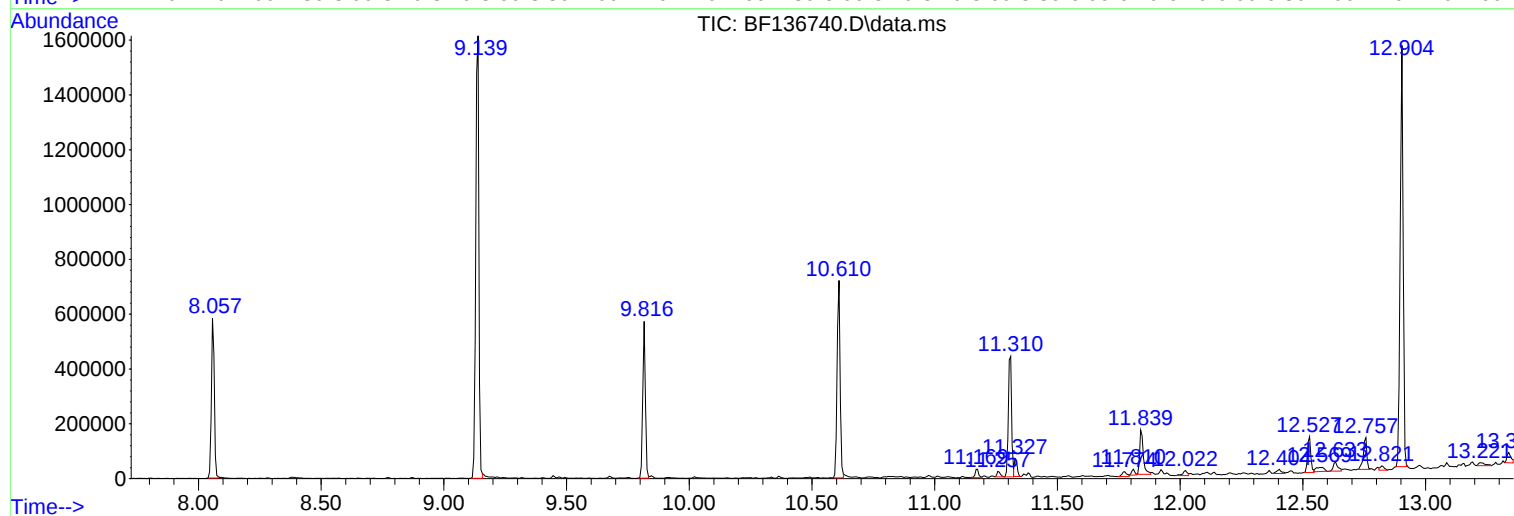
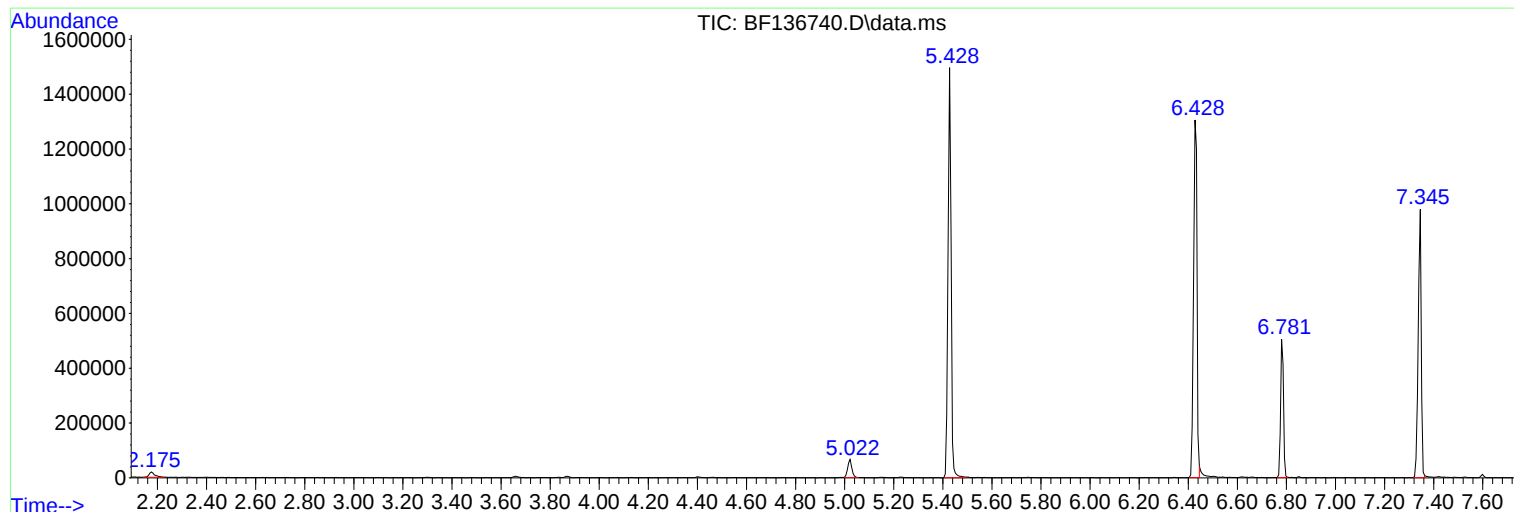
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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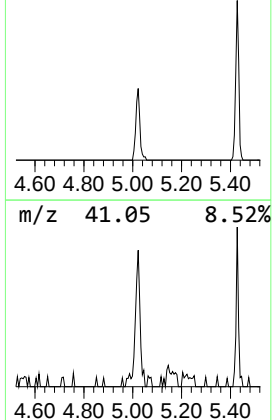
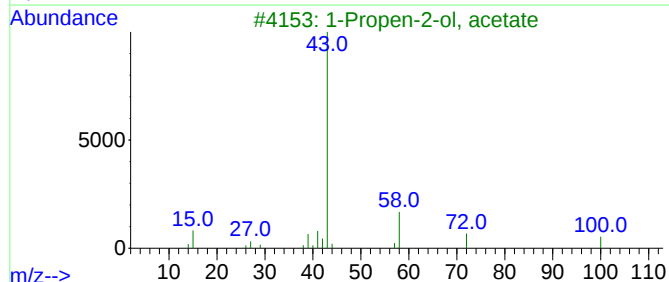
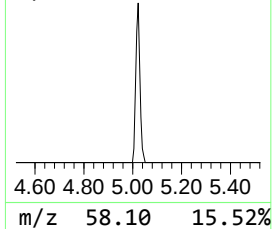
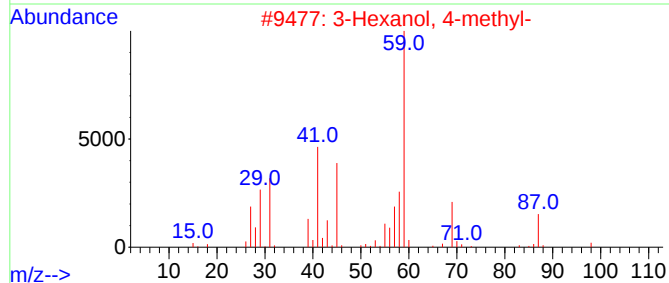
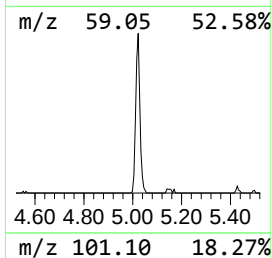
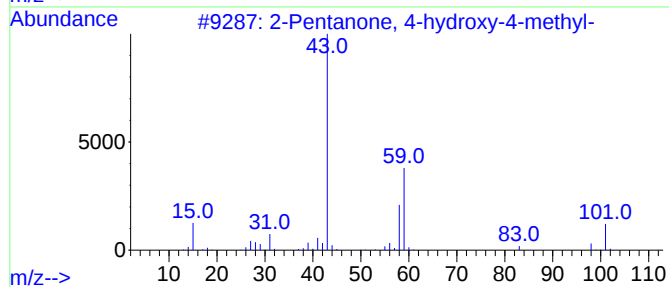
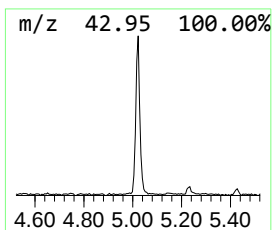
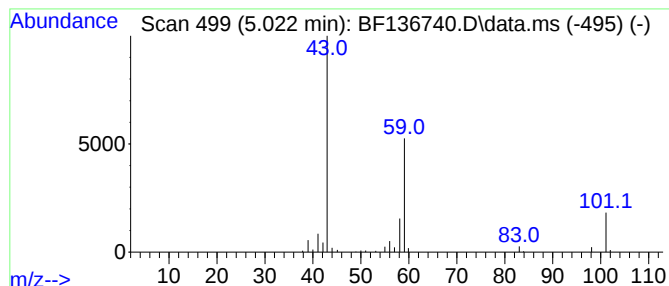
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	3.78 ng	77754	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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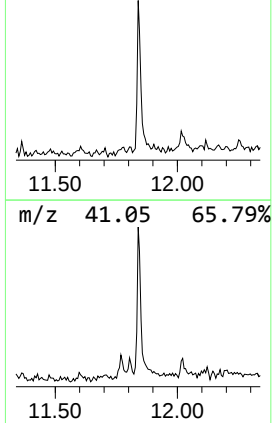
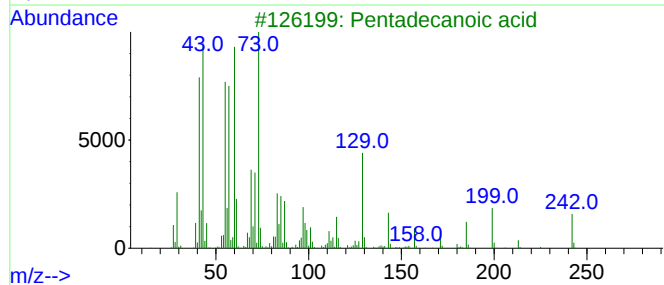
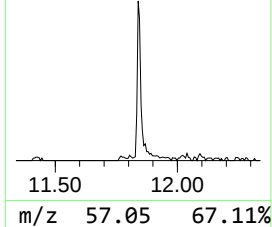
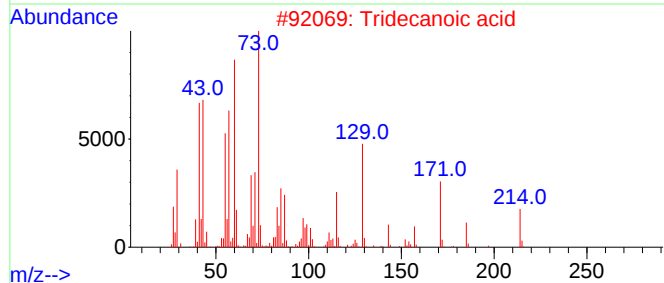
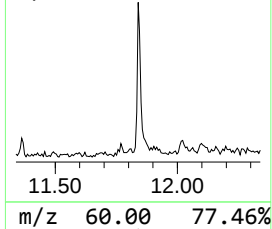
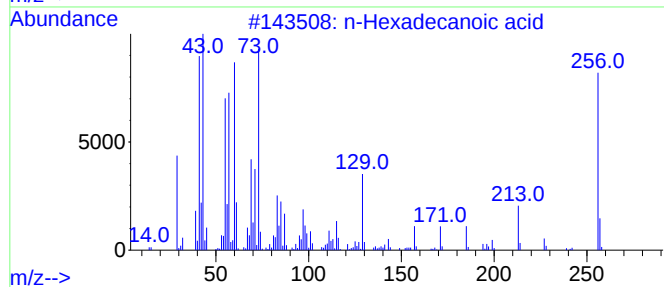
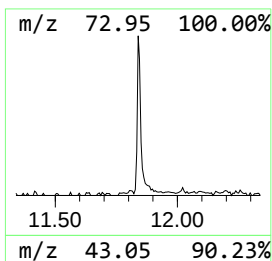
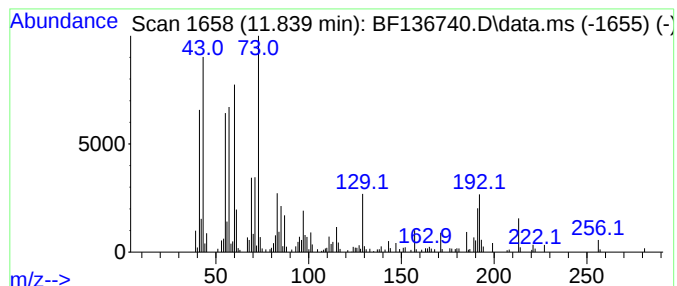
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	8.08 ng	166153	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	78
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			Undecanoic acid	186	C11H22O2	000112-37-8	50
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	49



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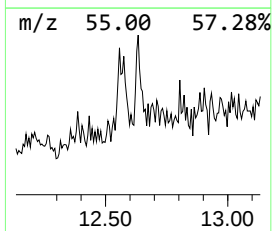
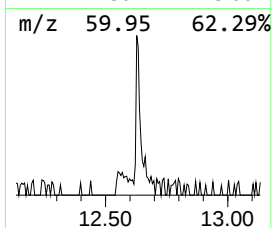
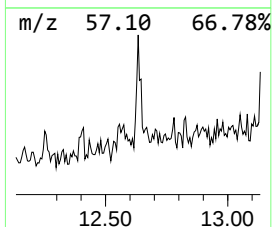
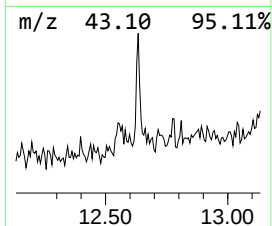
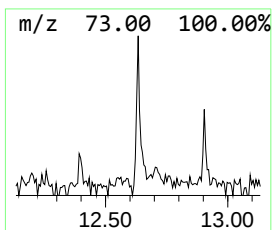
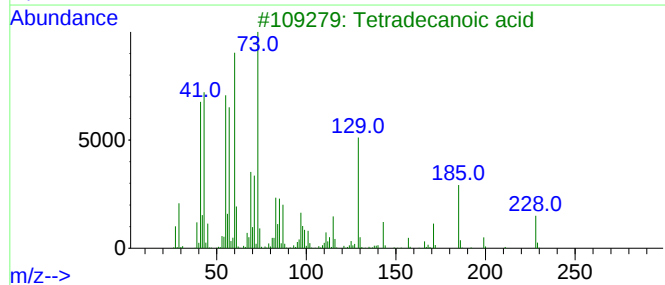
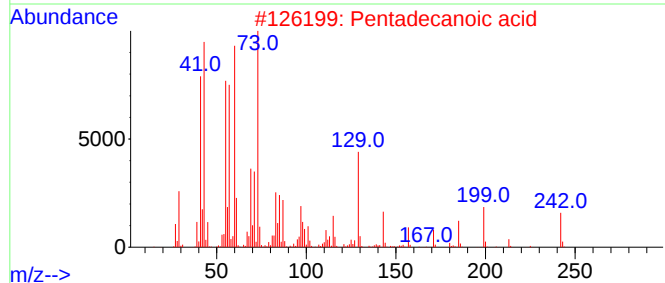
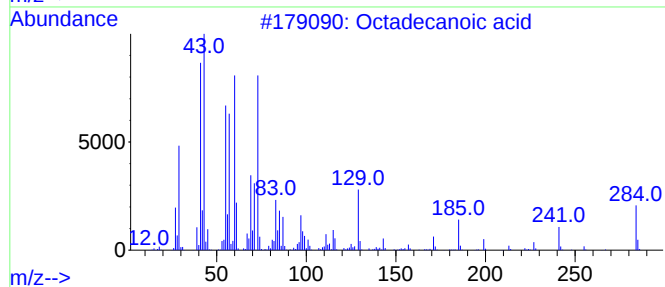
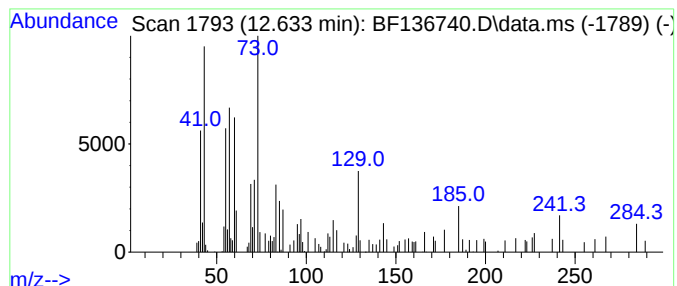
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.11 ng	43323	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	49
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47



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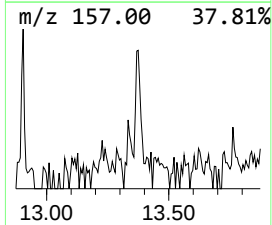
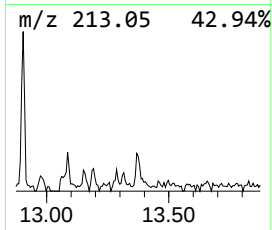
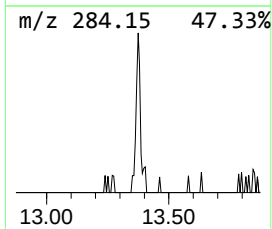
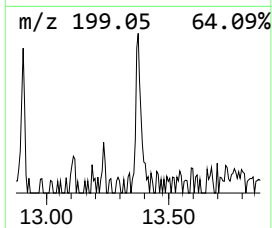
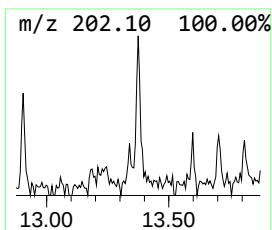
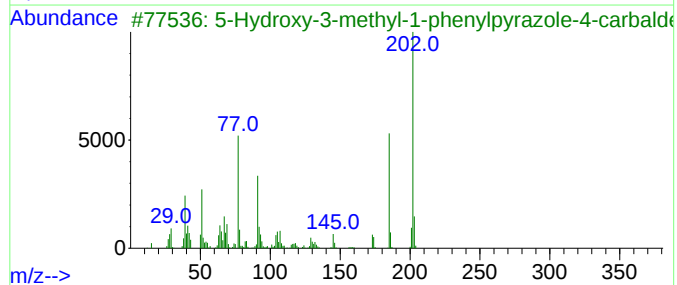
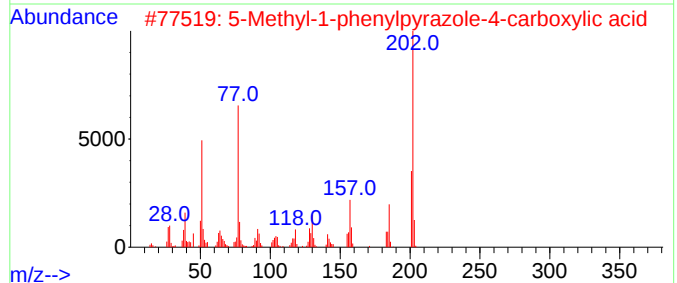
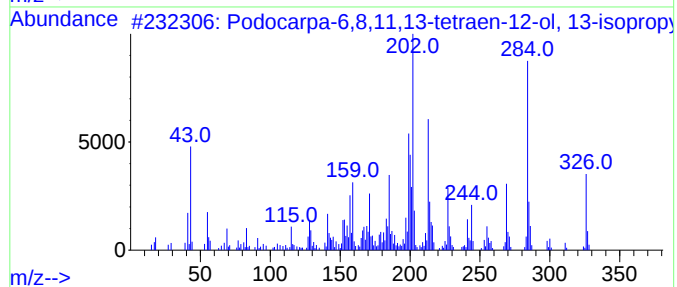
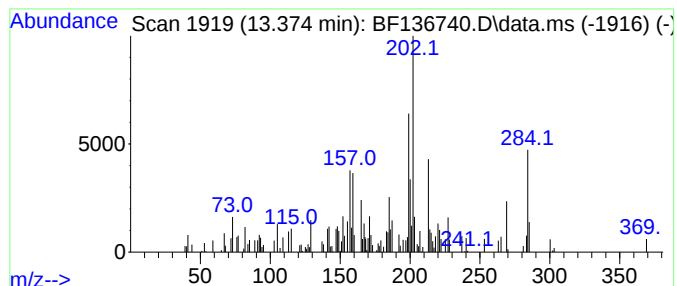
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown13.374 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.374	2.38 ng	59849	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Podocarpa-6,8,11,13-tetraen-12-o...	326	C22H30O2	022160-86-7	43
2			5-Methyl-1-phenylpyrazole-4-carb...	202	C11H10N2O2	091138-00-0	25
3			5-Hydroxy-3-methyl-1-phenylpyraz...	202	C11H10N2O2	060484-29-9	25
4			Fluoren-9-one, 9a-hydroxy-1,2,3,...	202	C13H14O2	1000160-37-9	25
5			2-Naphthoic acid, 6-methoxy-	202	C12H10O3	002471-70-7	22



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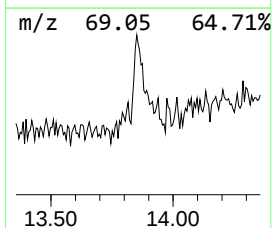
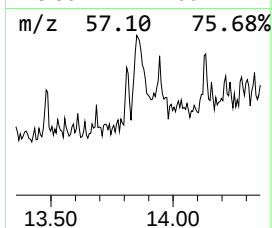
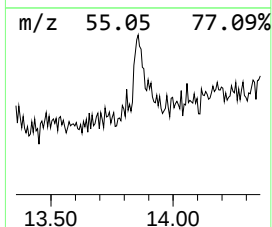
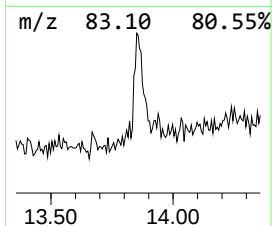
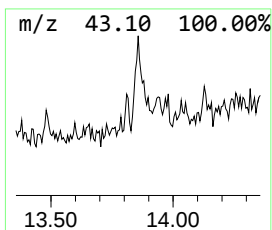
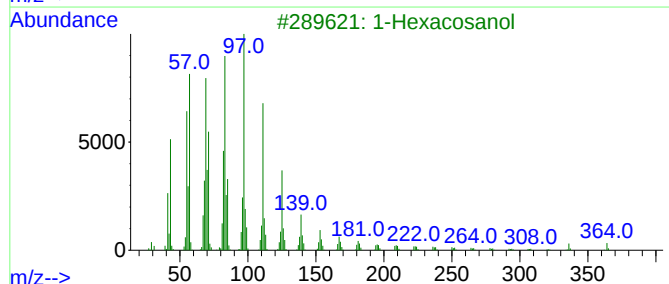
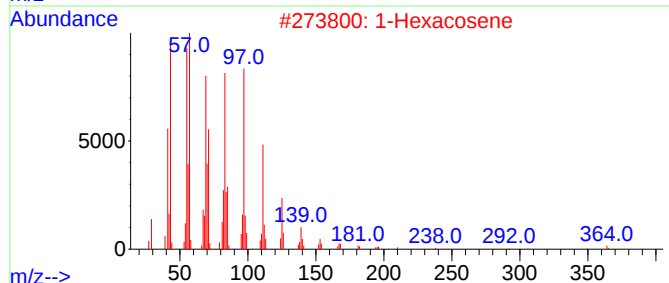
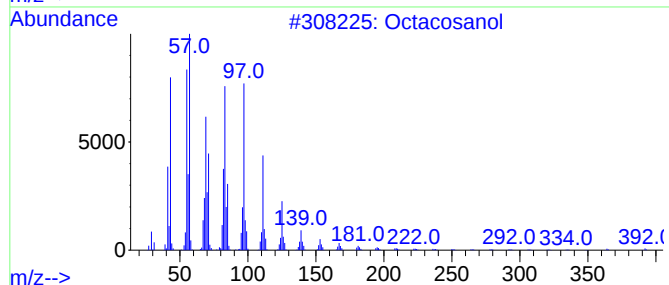
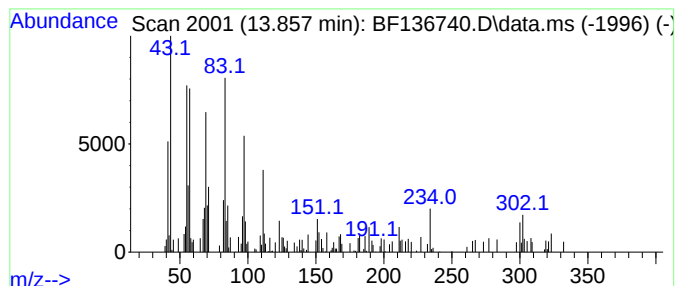
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Peak Number 5 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.51 ng	63187	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	60
2			1-Hexacosene	364	C26H52	018835-33-1	60
3			1-Hexacosanol	382	C26H54O	000506-52-5	53
4			Heptacosyl acetate	438	C29H58O2	1000351-78-2	53
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136740.D
Acq On : 27 Dec 2023 02:12
Operator : CG\JU
Sample : 05602-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-1

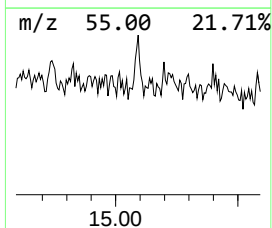
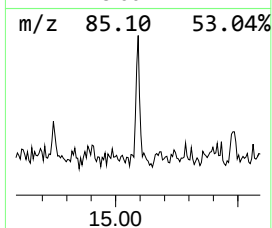
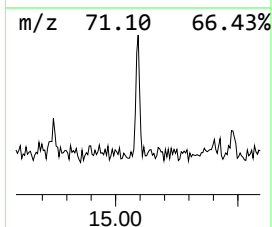
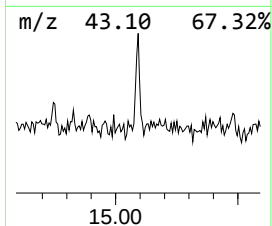
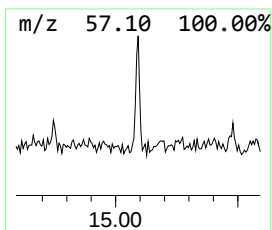
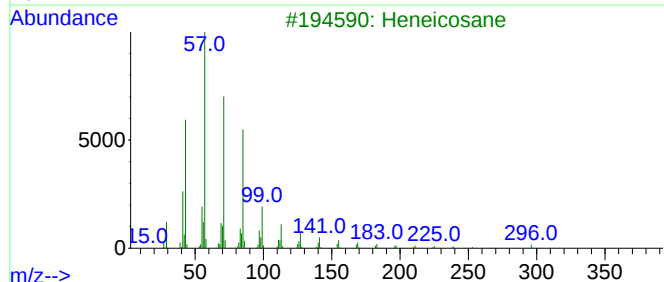
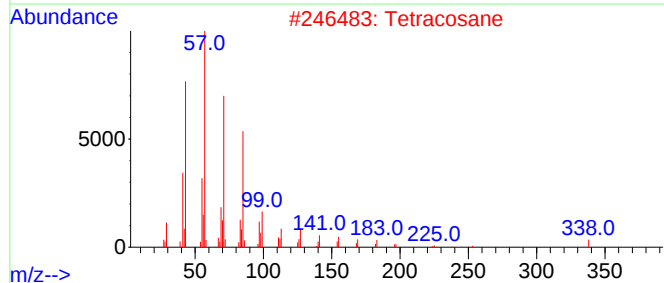
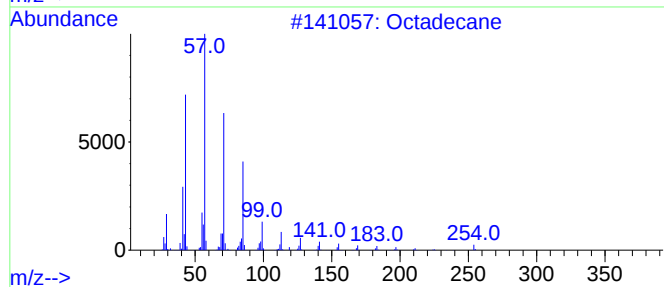
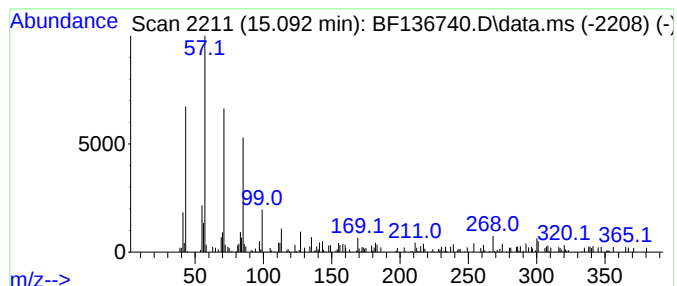
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.84 ng	37933	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	94
2			Tetracosane	338	C24H50	000646-31-1	91
3			Heneicosane	296	C21H44	000629-94-7	89
4			Docosane	310	C22H46	000629-97-0	89
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136740.D
Acq On : 27 Dec 2023 02:12
Operator : CG\JU
Sample : 05602-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-Pentanone, 4-...	5.022	3.8	ng	77754	1	6.781	411370	20.0
n-Hexadecanoic ...	11.839	8.1	ng	166153	4	11.310	411424	20.0
Octadecanoic acid	12.633	2.1	ng	43323	4	11.310	411424	20.0
unknown13.374	13.374	2.4	ng	59849	5	13.963	503209	20.0
Octacosanol	13.857	2.5	ng	63187	5	13.963	503209	20.0
Octadecane	15.092	2.8	ng	37933	6	15.439	267332	20.0