

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
 Data File : BF135033.D
 Acq On : 31 Aug 2023 06:36
 Operator : CG\JU
 Sample : 04183-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-02-082523

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135033.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.398	559	563	567	rBV	2152043	1986850	100.00%	11.413%
2	6.410	730	735	738	rBV	2113713	1919735	96.62%	11.028%
3	6.769	793	796	800	rBV	843909	769429	38.73%	4.420%
4	7.334	887	892	895	rBV	1434220	1207375	60.77%	6.936%
5	8.051	1008	1014	1017	rBV	1192831	975663	49.11%	5.605%
6	9.128	1193	1197	1201	rBV	2092452	1800862	90.64%	10.345%
7	9.251	1214	1218	1220	rBV	26388	26976	1.36%	0.155%
8	9.810	1309	1313	1316	rVB	1027565	857144	43.14%	4.924%
9	10.245	1384	1387	1390	rBV	25753	23213	1.17%	0.133%
10	10.469	1423	1425	1430	rVB	21011	22079	1.11%	0.127%
11	10.598	1443	1447	1451	rBV	1113539	950319	47.83%	5.459%
12	10.722	1466	1468	1476	rVB2	56815	76991	3.88%	0.442%
13	11.175	1543	1545	1547	rBV	59116	44782	2.25%	0.257%
14	11.204	1547	1550	1554	rVB	44850	48814	2.46%	0.280%
15	11.304	1563	1567	1569	rBV	810372	745153	37.50%	4.280%
16	11.327	1569	1571	1574	rVV	106006	86904	4.37%	0.499%
17	11.375	1577	1579	1583	rVB	29596	25750	1.30%	0.148%
18	11.604	1615	1618	1621	rBV	62007	48571	2.44%	0.279%
19	11.704	1632	1635	1640	rVB	177284	153911	7.75%	0.884%
20	11.839	1655	1658	1667	rBV2	262662	261434	13.16%	1.502%
21	11.916	1669	1671	1674	rVV2	26264	23286	1.17%	0.134%
22	12.016	1685	1688	1691	rVB	57682	45281	2.28%	0.260%
23	12.363	1744	1747	1749	rBV	26270	24900	1.25%	0.143%
24	12.398	1749	1753	1755	rBV	1342819	1213721	61.09%	6.972%
25	12.422	1755	1757	1759	rVB	742016	601286	30.26%	3.454%
26	12.504	1768	1771	1772	rBV	166029	132702	6.68%	0.762%
27	12.522	1772	1774	1778	rVB	140193	144345	7.27%	0.829%
28	12.633	1790	1793	1798	rBV3	65437	76045	3.83%	0.437%
29	12.751	1808	1813	1816	rBV	186881	177066	8.91%	1.017%
30	12.780	1816	1818	1821	rVB	65868	47250	2.38%	0.271%
31	12.898	1835	1838	1842	rBV	1435508	1294442	65.15%	7.436%
32	13.139	1877	1879	1884	rVB2	74976	81168	4.09%	0.466%
33	13.486	1936	1938	1941	rBV	60050	50010	2.52%	0.287%
34	13.816	1991	1994	2001	rVB2	127597	160992	8.10%	0.925%
35	13.957	2014	2018	2021	rBV	750981	754990	38.00%	4.337%
36	13.986	2021	2023	2025	rVB	68351	54619	2.75%	0.314%

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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-BF083023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.445	2099	2101	2104	rBV2	66783	60784	3.06%	0.349%
38	15.427	2265	2268	2275	rVB	349882	433365	21.81%	2.489%

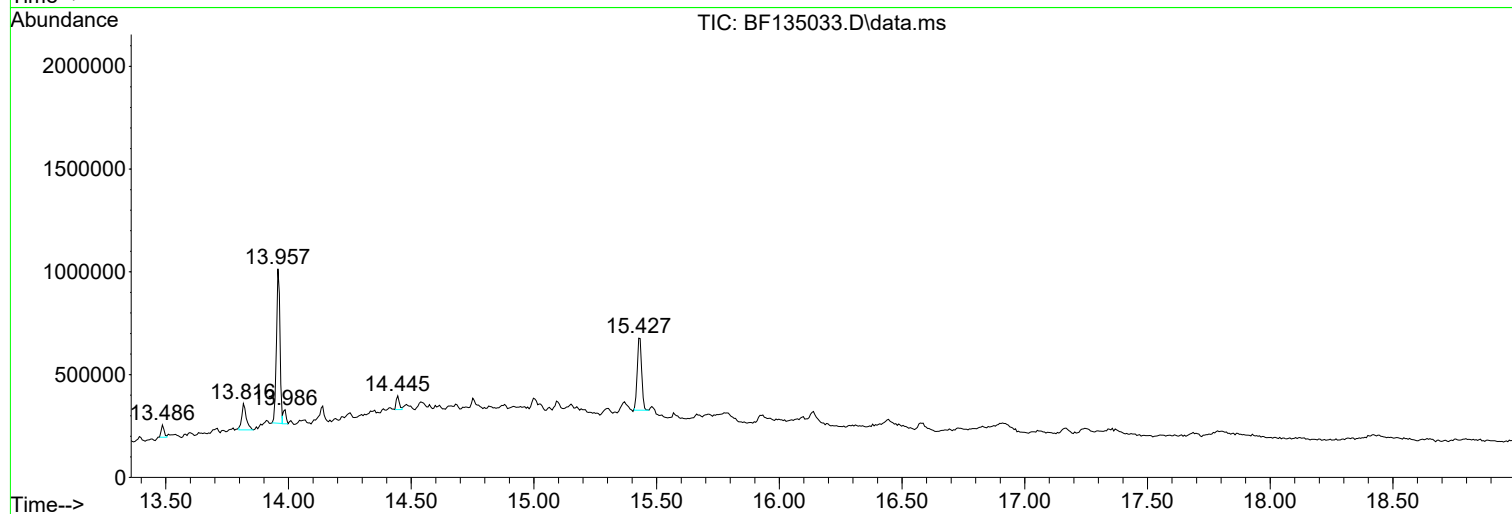
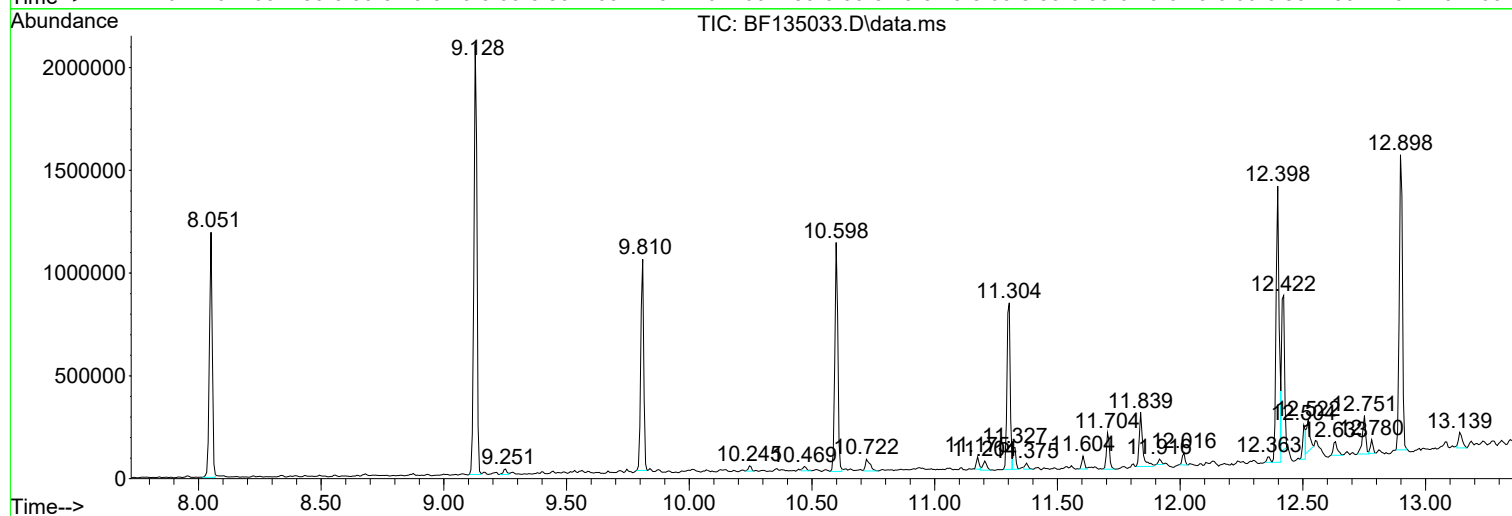
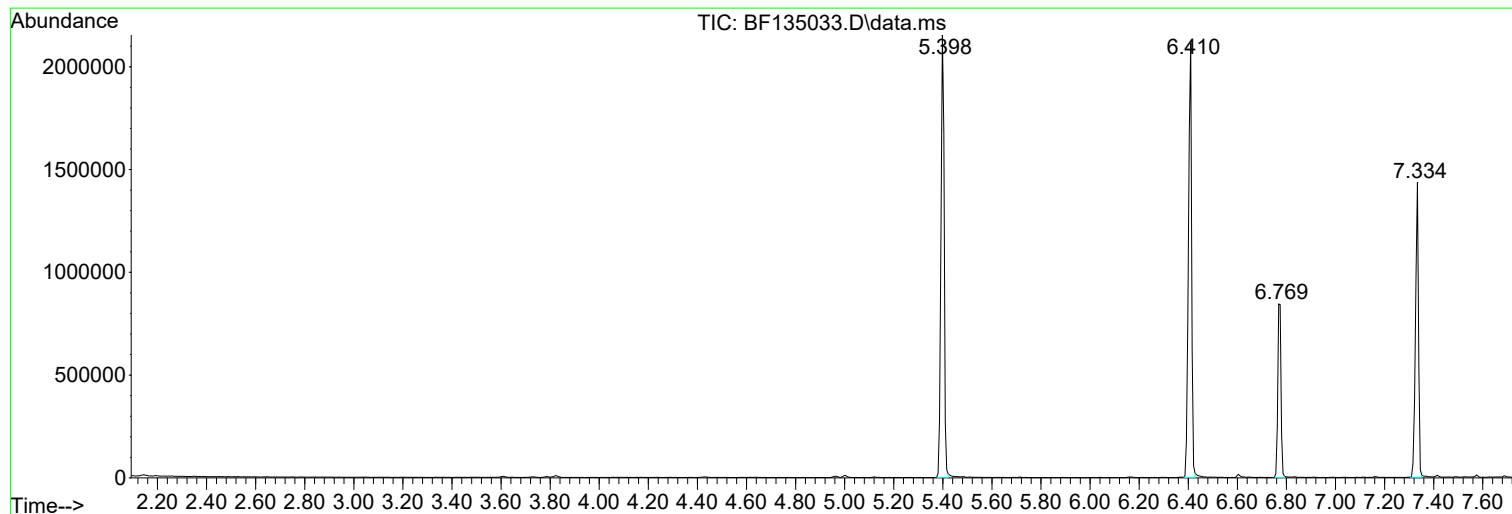
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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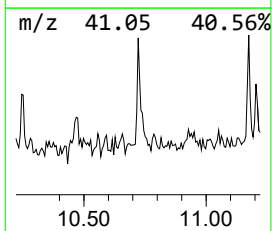
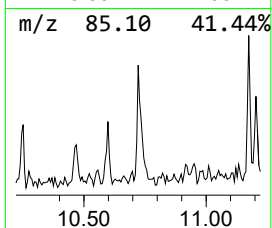
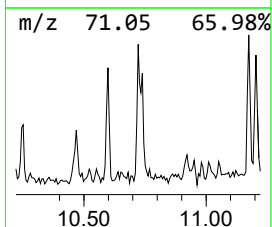
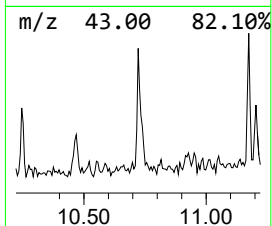
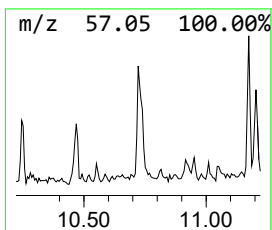
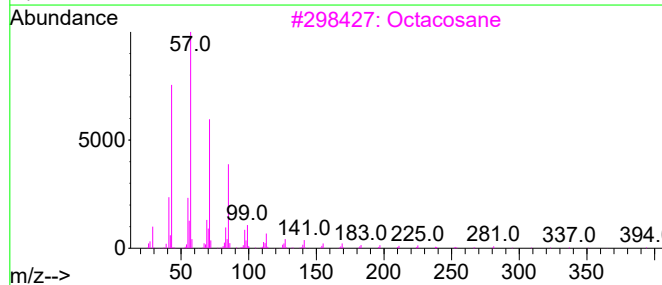
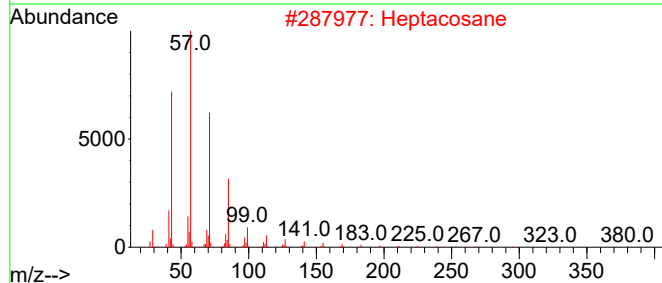
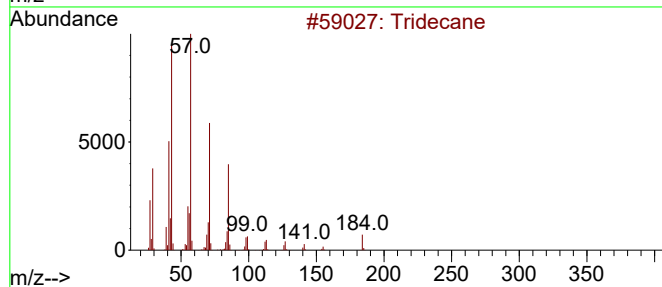
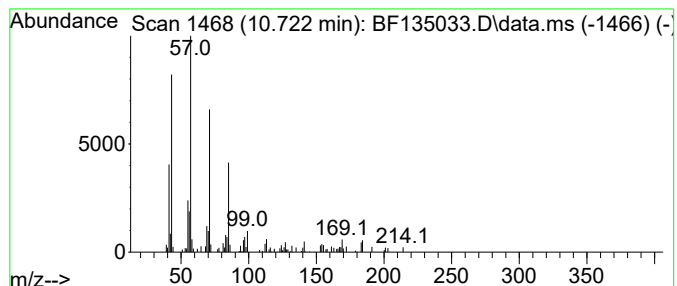
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.722	2.07 ng	76991	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	91
2			Heptacosane	380	C27H56	000593-49-7	83
3			Octacosane	394	C28H58	000630-02-4	83
4			Dodecane	170	C12H26	000112-40-3	83
5			Nonadecane	268	C19H40	000629-92-5	80



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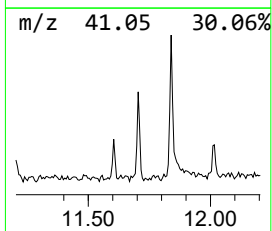
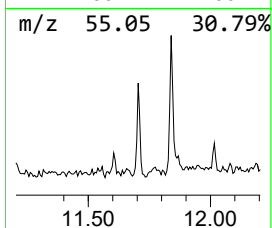
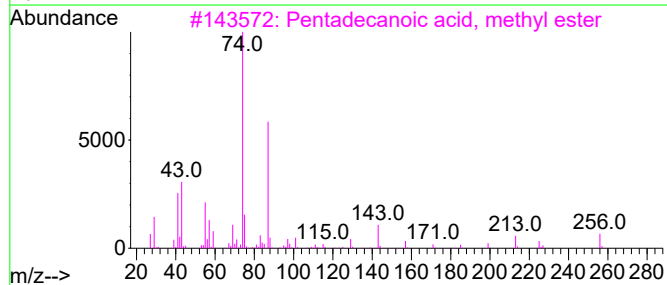
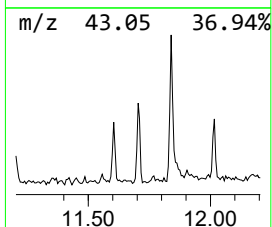
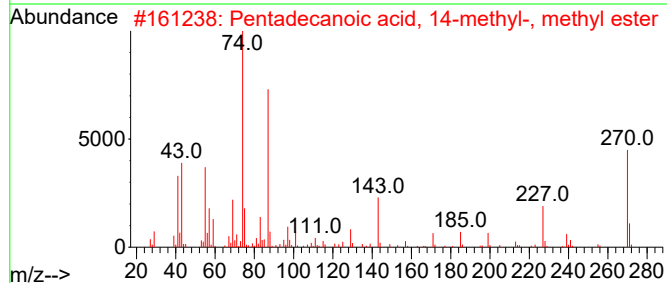
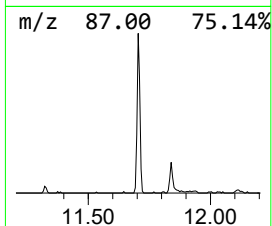
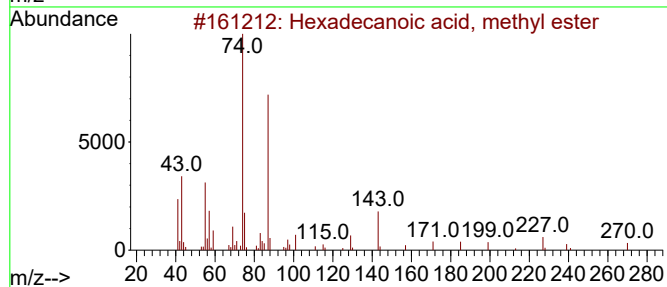
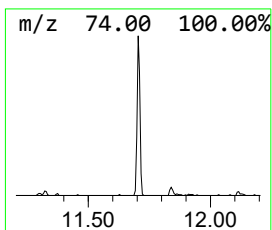
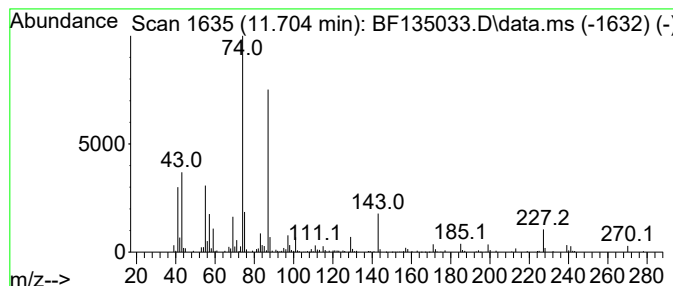
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.704	4.13 ng	153911	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	86
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86



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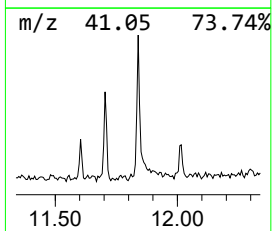
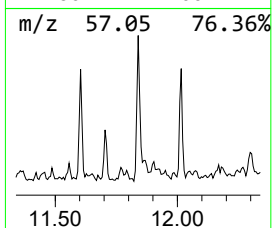
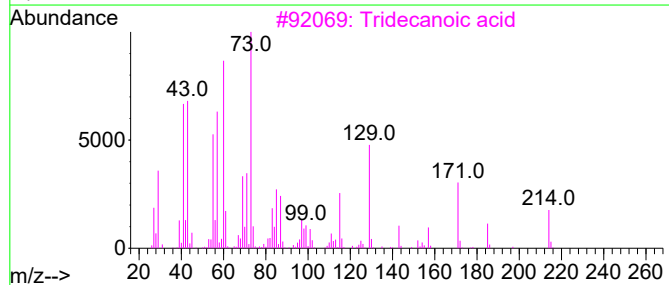
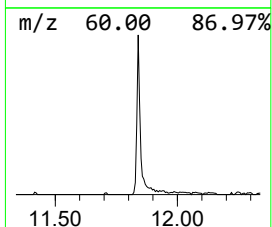
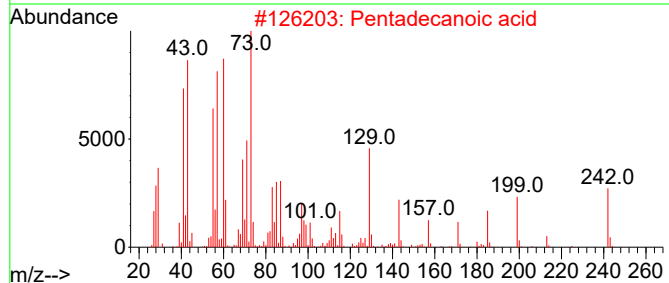
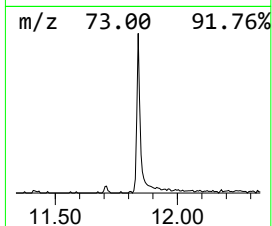
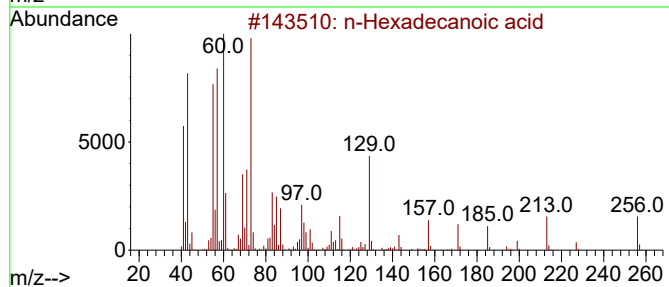
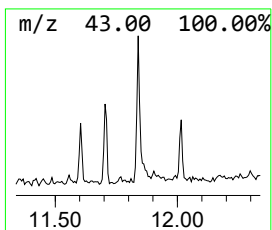
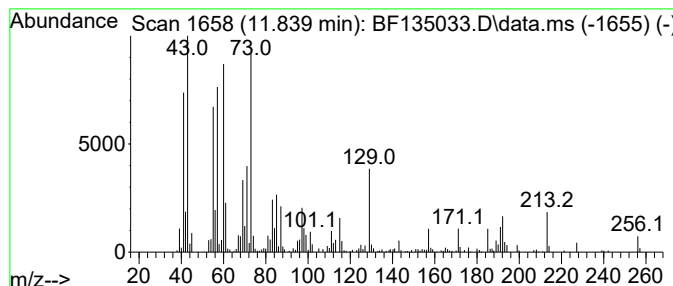
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	7.02 ng	261434	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	58



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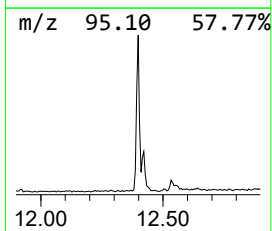
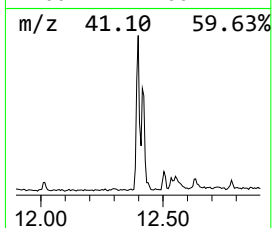
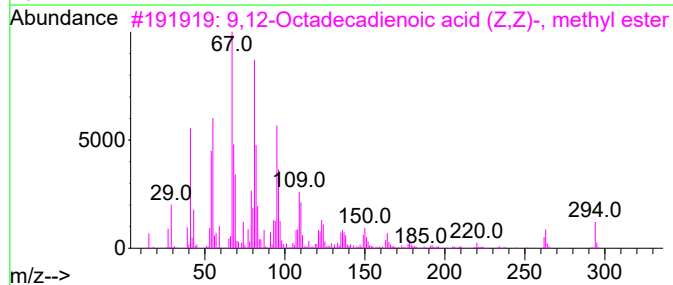
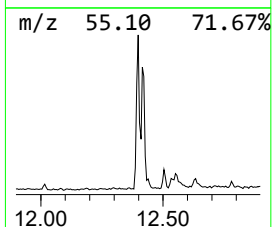
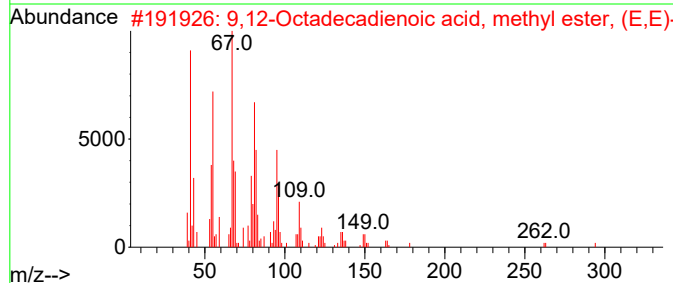
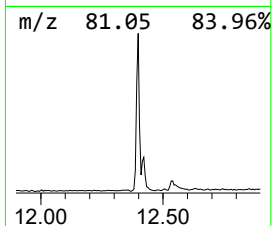
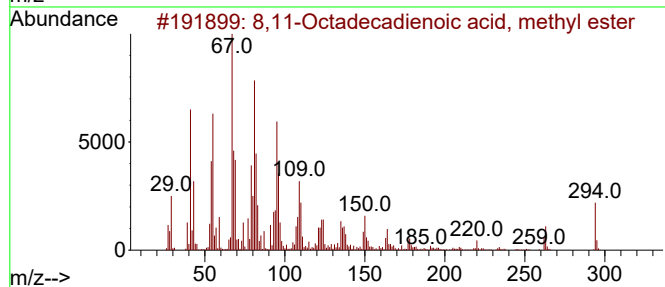
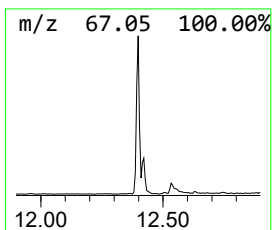
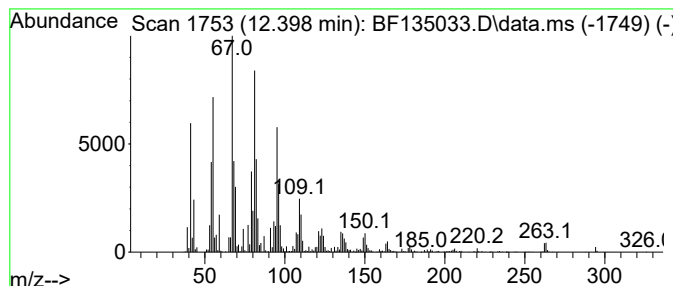
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 8,11-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.398	32.58 ng	1213720	Phenanthrene-d10		11.304	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	8,11-Octadecadienoic acid, methy...		294	C19H34O2	056599-58-7	99
2	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002566-97-4	99
3	9,12-Octadecadienoic acid (Z,Z)-...		294	C19H34O2	000112-63-0	99
4	10,13-Octadecadienoic acid, meth...		294	C19H34O2	056554-62-2	99
5	9,15-Octadecadienoic acid, methy...		294	C19H34O2	017309-05-6	99



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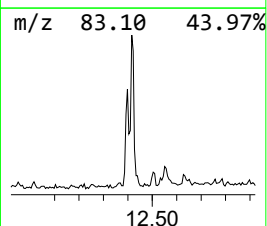
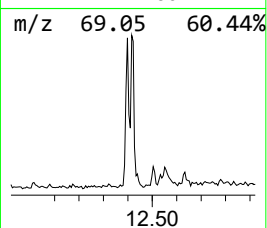
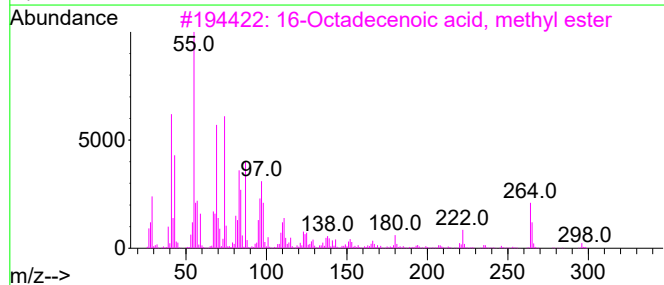
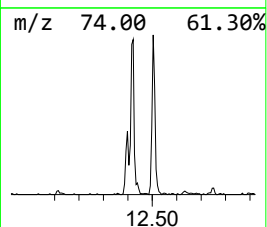
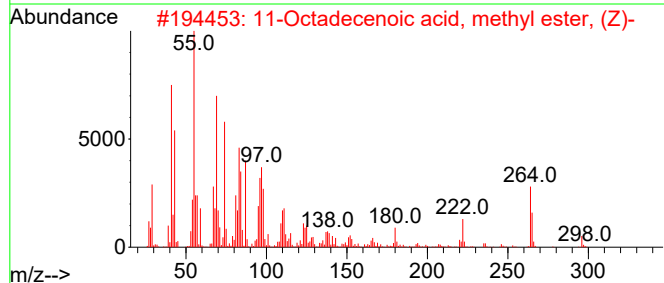
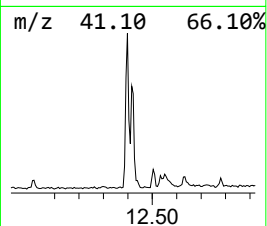
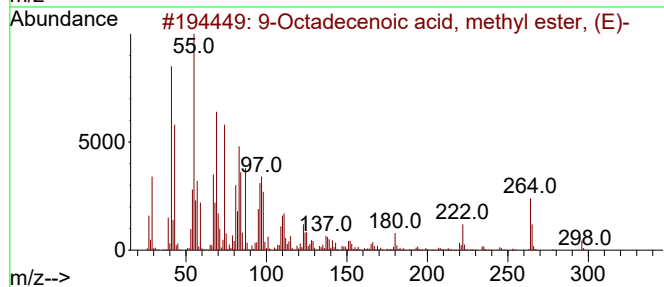
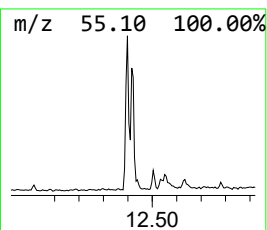
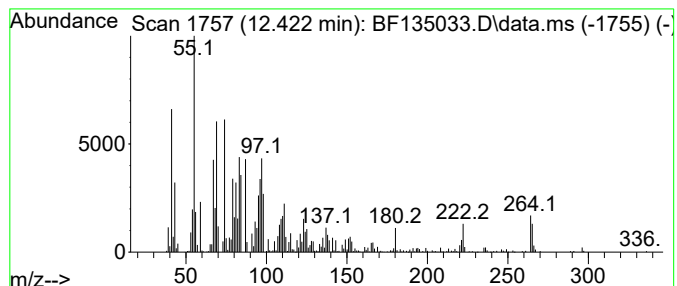
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.422	16.14 ng	601286	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4			6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99
5			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135033.D
Acq On : 31 Aug 2023 06:36
Operator : CG\JU
Sample : 04183-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-082523

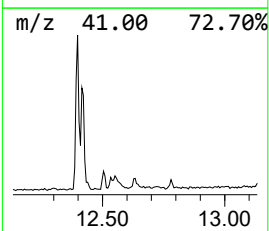
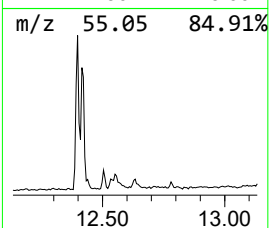
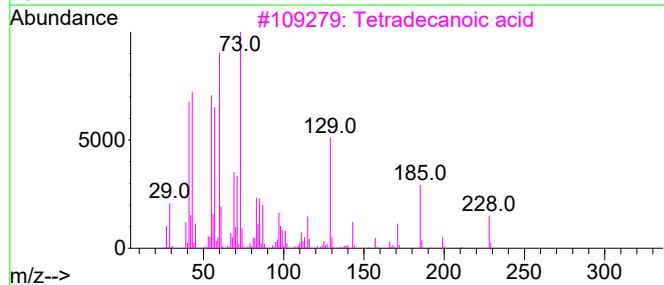
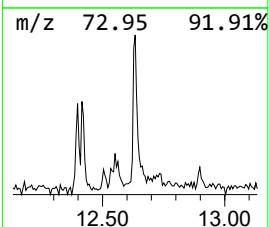
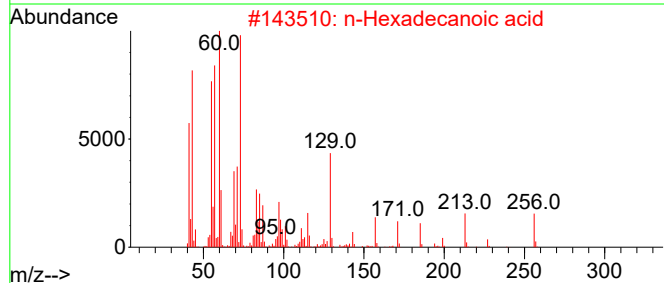
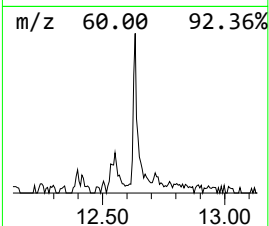
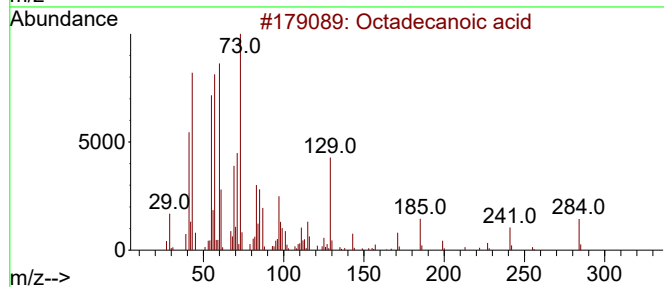
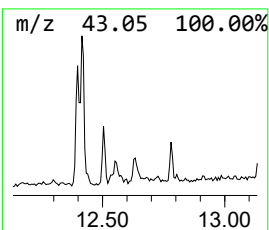
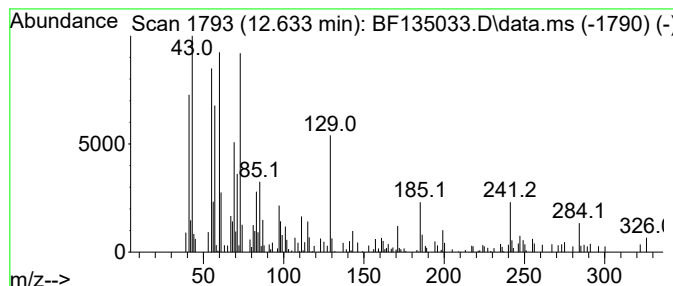
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.01 ng	76045	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			Undecanoic acid	186	C11H22O2	000112-37-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135033.D
Acq On : 31 Aug 2023 06:36
Operator : CG\JU
Sample : 04183-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-082523

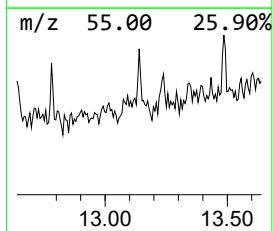
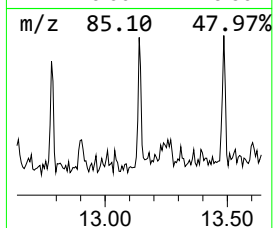
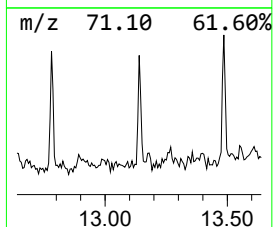
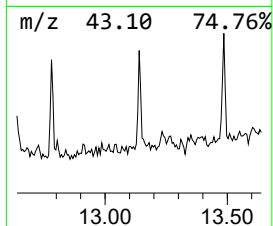
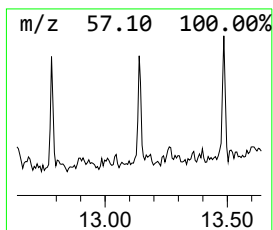
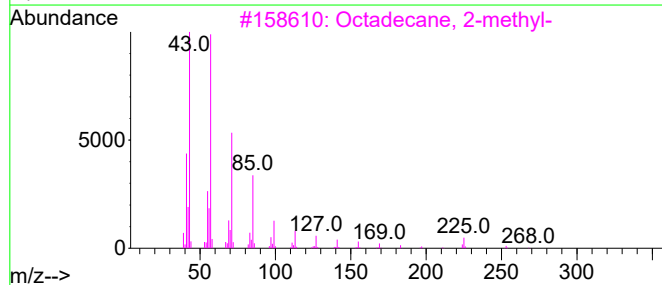
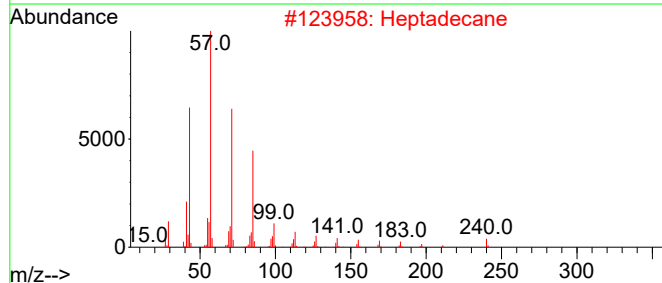
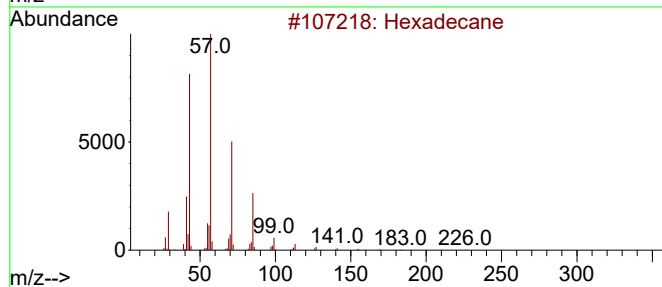
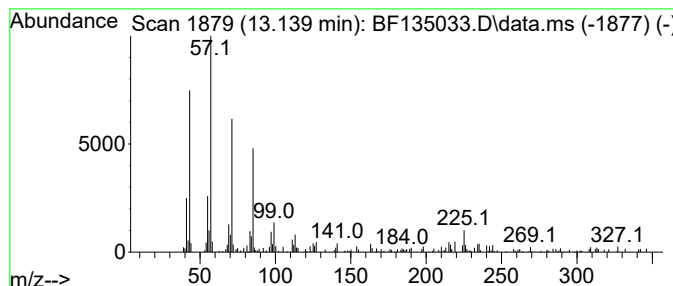
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	2.15 ng	81168	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	95
2			Heptadecane	240	C17H36	000629-78-7	89
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	83
4			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	74
5			Octacosane	394	C28H58	000630-02-4	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135033.D
Acq On : 31 Aug 2023 06:36
Operator : CG\JU
Sample : 04183-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-082523

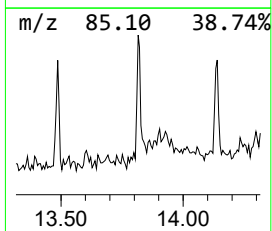
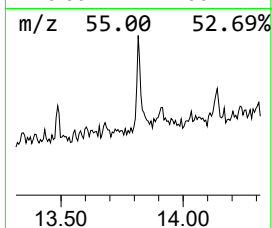
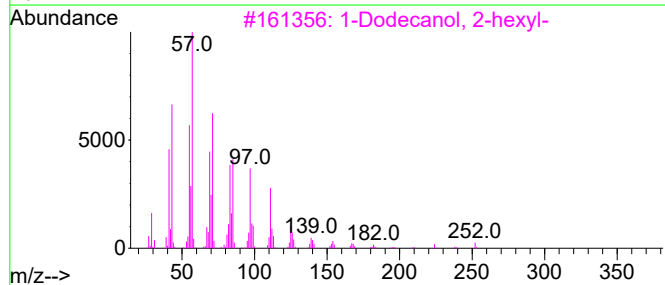
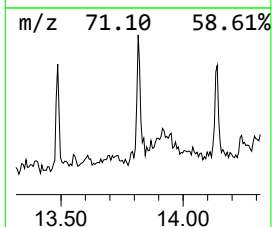
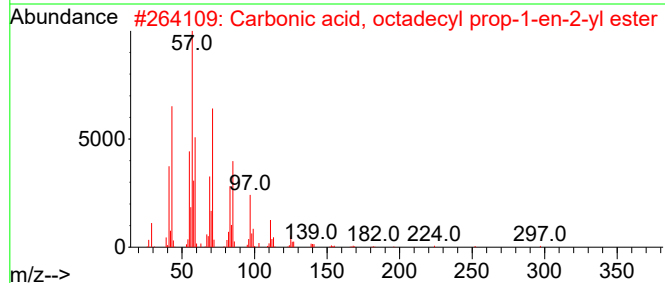
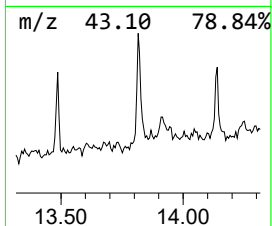
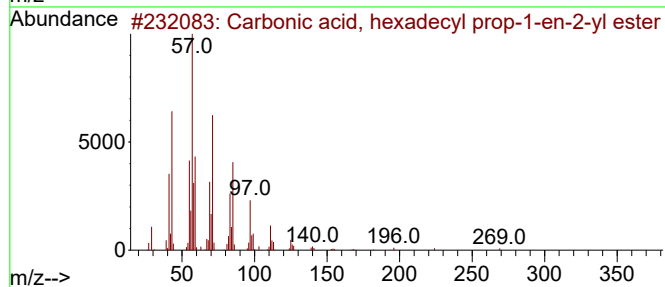
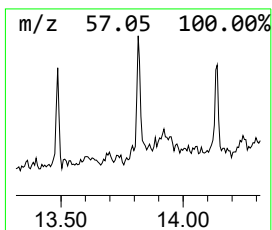
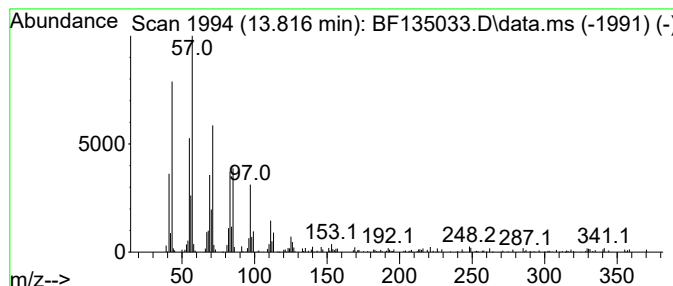
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Carbonic acid, hexadecyl pr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	4.26 ng	160992	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91
4			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	90
5			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135033.D
Acq On : 31 Aug 2023 06:36
Operator : CG\JU
Sample : 04183-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-082523

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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
Tridecane	10.722	2.1	ng	76991	4	11.304	745153	20.0
Hexadecanoic ac...	11.704	4.1	ng	153911	4	11.304	745153	20.0
n-Hexadecanoic ...	11.839	7.0	ng	261434	4	11.304	745153	20.0
8,11-Octadecadi...	12.398	32.6	ng	1213720	4	11.304	745153	20.0
9-Octadecenoic ...	12.422	16.1	ng	601286	4	11.304	745153	20.0
Octadecanoic acid	12.633	2.0	ng	76045	5	13.957	754990	20.0
Hexadecane	13.139	2.1	ng	81168	5	13.957	754990	20.0
Carbonic acid, ...	13.816	4.3	ng	160992	5	13.957	754990	20.0