LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090123\
Data File : BF135082.D
Acq On : 01 Sep 2023 18:14
Operator : CG\JU
Sample : 04202-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-3

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: BF135082.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	18	rVB	32151	44444	2.13%	0.275%
2	4.998	491	495	501	rVB	64035	76890	3.69%	0.475%
3	5.398	559	563	566	rBV	2081537	1876719	90.08%	11.599%
4	6.404	730	734	738	rBV	1799319	1859373	89.25%	11.491%
5	6.769	793	796	800	rBV	772546	595879	28.60%	3.683%
6	7.334	887	892	895	rBV	1287927	1209721	58.06%	7.476%
7	8.045	1009	1013	1017	rBV	862232	790828	37.96%	4.888%
8	9.128	1192	1197	1200	rBV	2531612	2083444	100.00%	12.876%
9	9.804	1308	1312	1316	rBV	1014826	819682	39.34%	5.066%
10	10.598	1443	1447	1450	rBV	1331868	1150071	55.20%	7.108%
11	11.298	1562	1566	1568	rBV	904780	738964	35.47%	4.567%
12	11.322	1568	1570	1573	rVV	121968	91476	4.39%	0.565%
13	11.369	1573	1578	1582	rVB	32239	34965	1.68%	0.216%
14	11.833	1654	1657	1662	rBV	203849	193322	9.28%	1.195%
15	11.910	1667	1670	1673	rBV	24014	26163	1.26%	0.162%
16	12.516	1769	1773	1777	rBV	168085	141592	6.80%	0.875%
17	12.627	1788	1792	1804	rBV5	40917	66584	3.20%	0.412%
18	12.745	1806	1812	1815	rBV2	148148	155635	7.47%	0.962%
19	12.898	1834	1838	1841	rVB	1735280	1621069	77.81%	10.019%
20	13.139	1875	1879	1882	rBV2	20775	28613	1.37%	0.177%
21	13.180	1882	1886	1889	rVB2	26988	26810	1.29%	0.166%
22	13.698	1969	1974	1976	rBV3	18538	25526	1.23%	0.158%
23	13.827	1988	1996	2009	rBV6	58409	173553	8.33%	1.073%
24	13.951	2012	2017	2020	rVV2	733417	734462	35.25%	4.539%
25	13.974	2020	2021	2024	rVB	84831	61493	2.95%	0.380%
26	14.127	2044	2047	2052	rBV2	34356	34126	1.64%	0.211%
27	14.339	2079	2083	2087	rBV	30375	35599	1.71%	0.220%
28	14.433	2093	2099	2103	rBV2	45875	54896	2.63%	0.339%
29	14.721	2144	2148	2158	rBV	228444	273730	13.14%	1.692%
30	14.992	2189	2194	2203	rBV	92644	179529	8.62%	1.110%
31	15.292	2240	2245	2251	rVB	56551	79135	3.80%	0.489%
32	15.351	2251	2255	2261	rBV	80831	105505	5.06%	0.652%
33	15.421	2261	2267	2271	rBV	501268	632642	30.37%	3.910%
34	15.904	2346	2349	2355	rBV5	16855	27963	1.34%	0.173%
35	16.033	2367	2371	2379	rVB9	10371	26930	1.29%	0.166%
36	16.892	2511	2517	2526	rVB3	31075	63593	3.05%	0.393%

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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	17.333	2587	2592	2601	rVB2	16949	39569	1.90%	0.245%

Sum of corrected areas: 16180495

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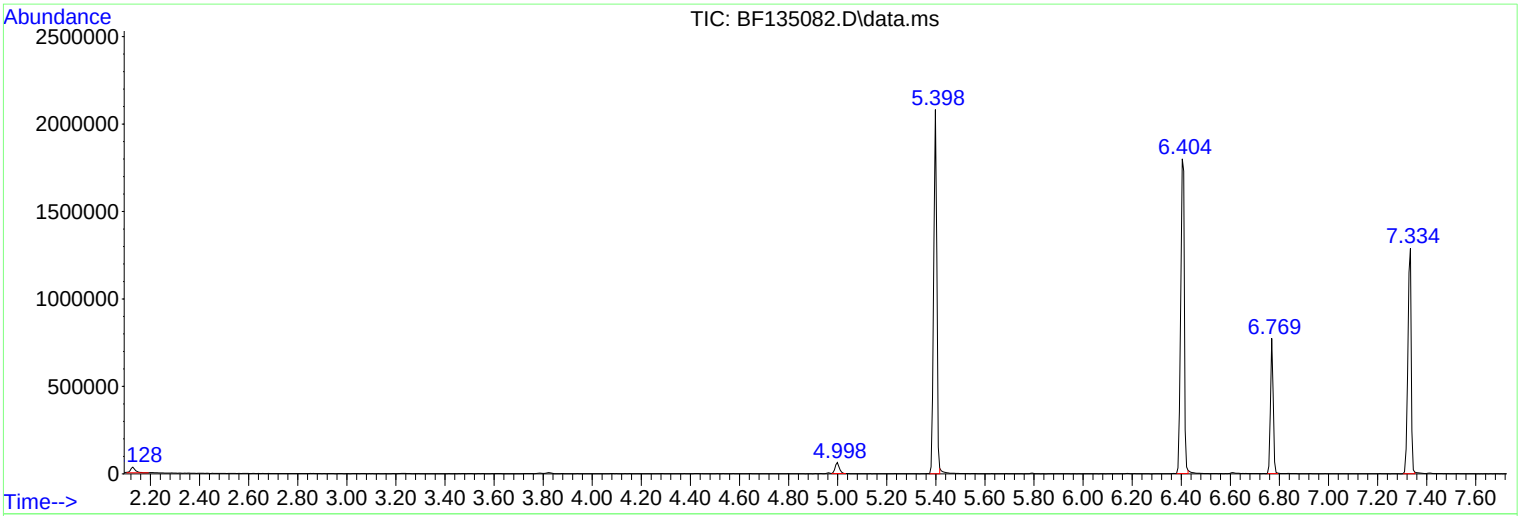
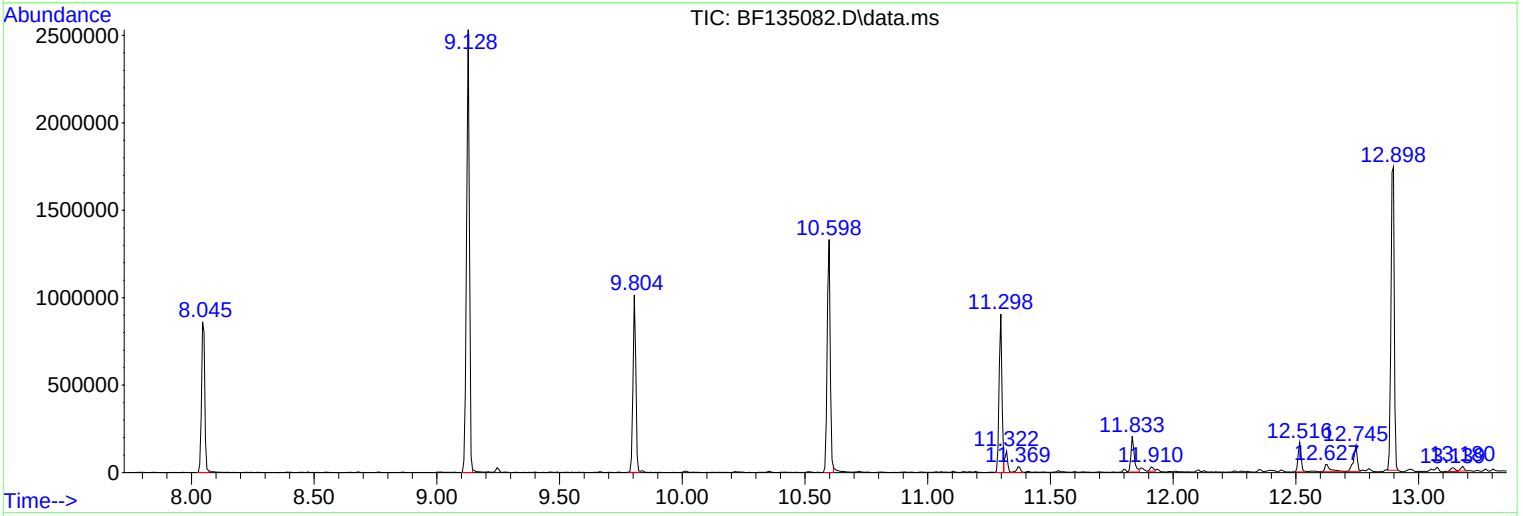
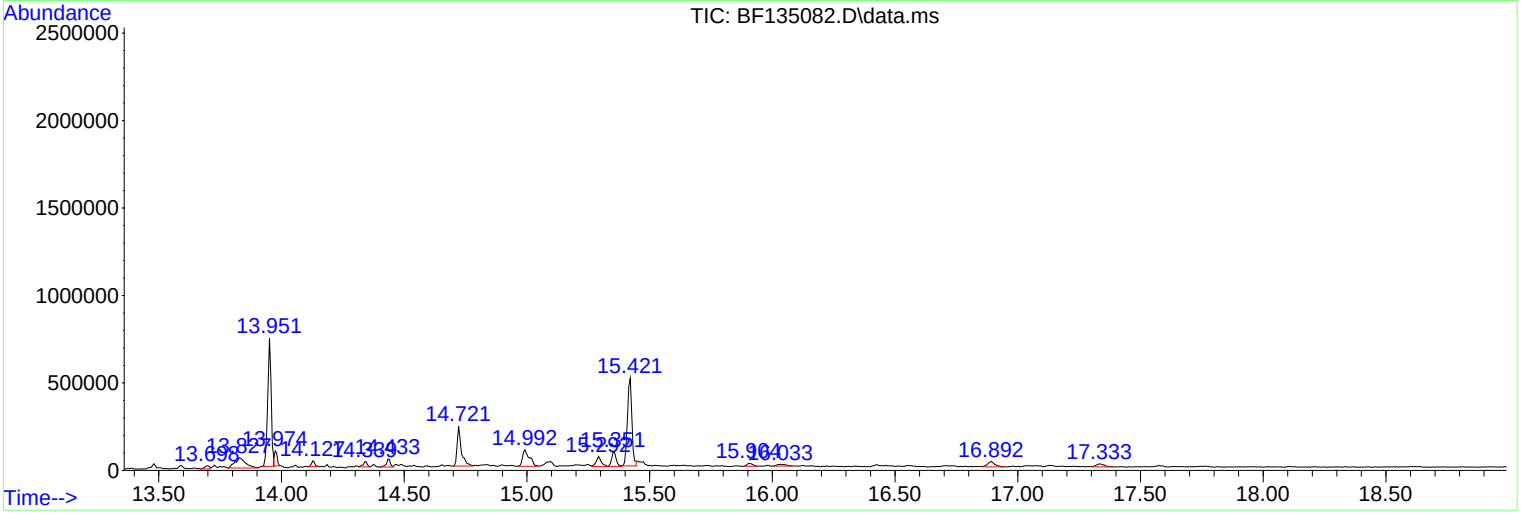
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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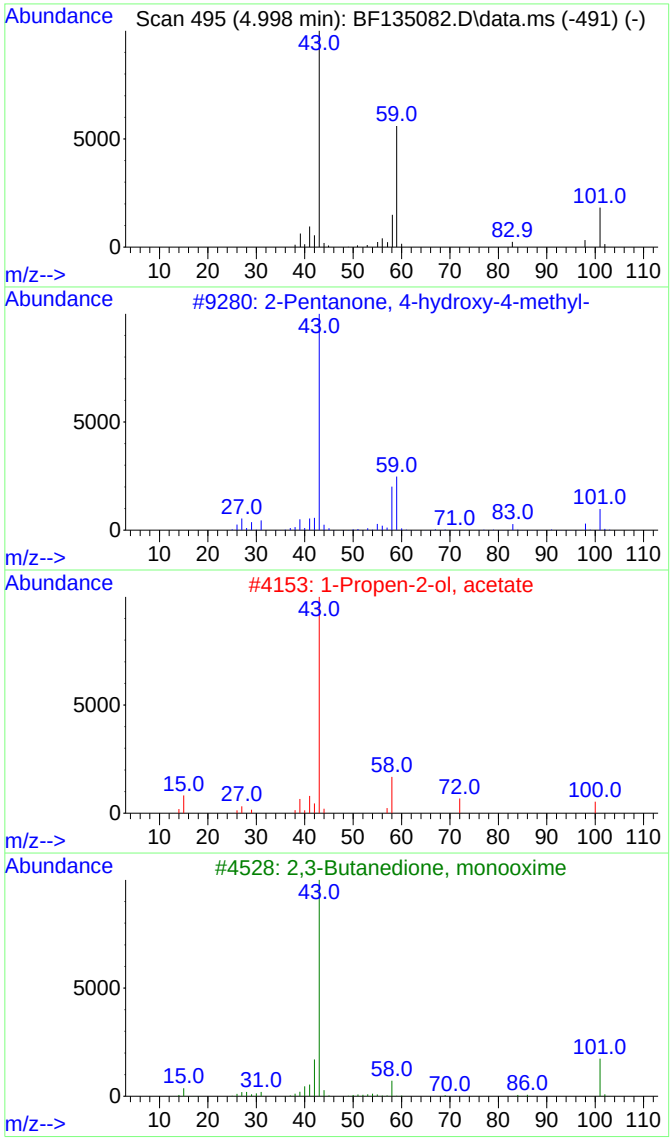
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

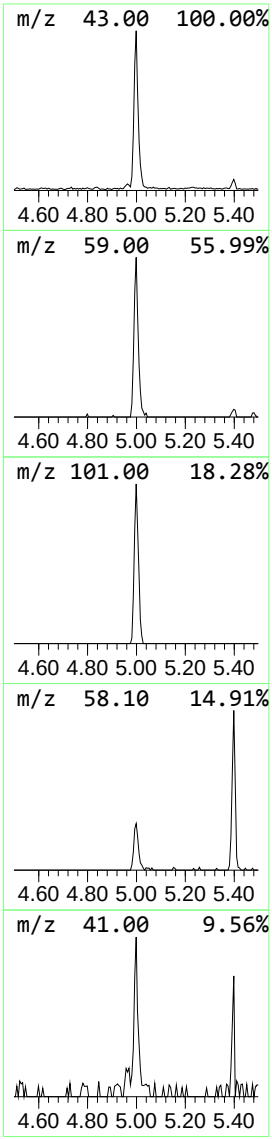
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	2.58 ng	76890	1,4-Dichlorobenzene-d4	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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

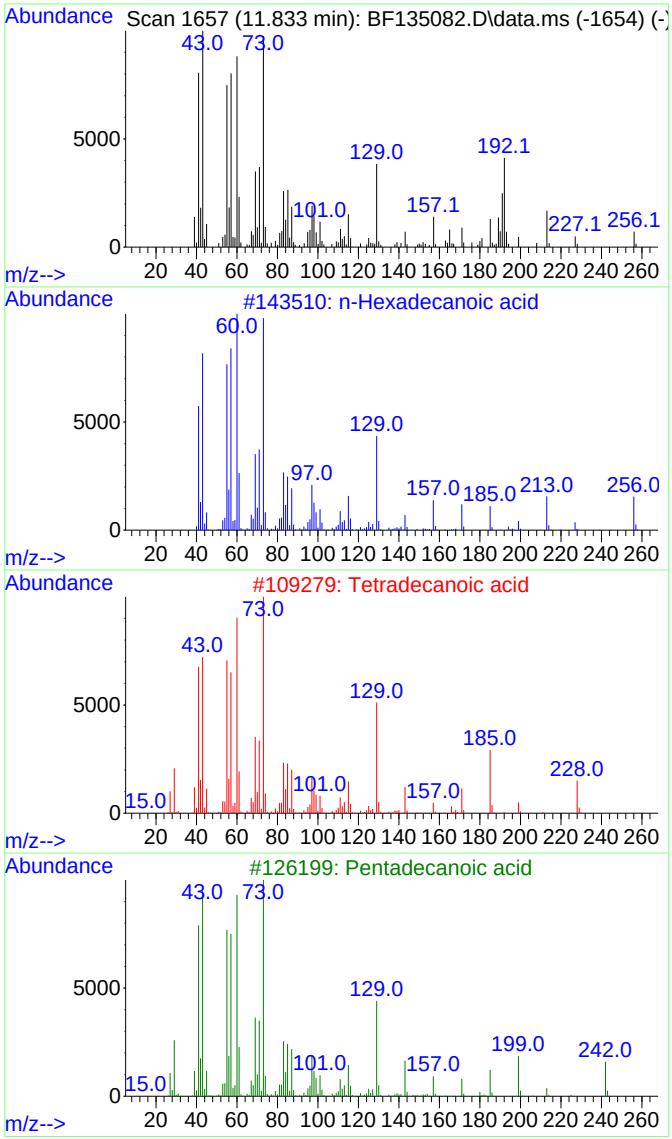
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

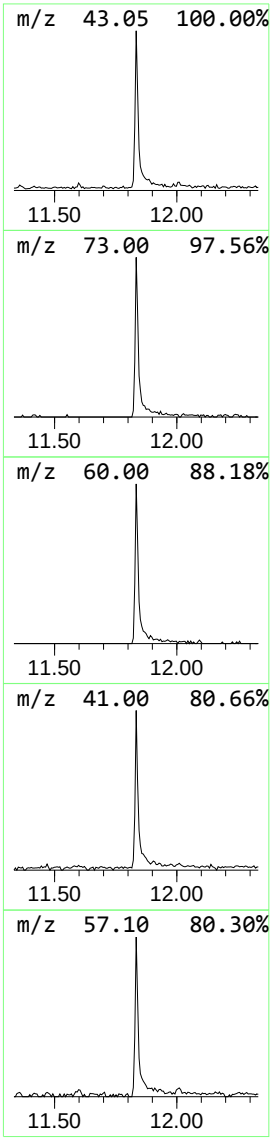
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	5.23 ng	193322	Phenanthrene-d10	11.298

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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

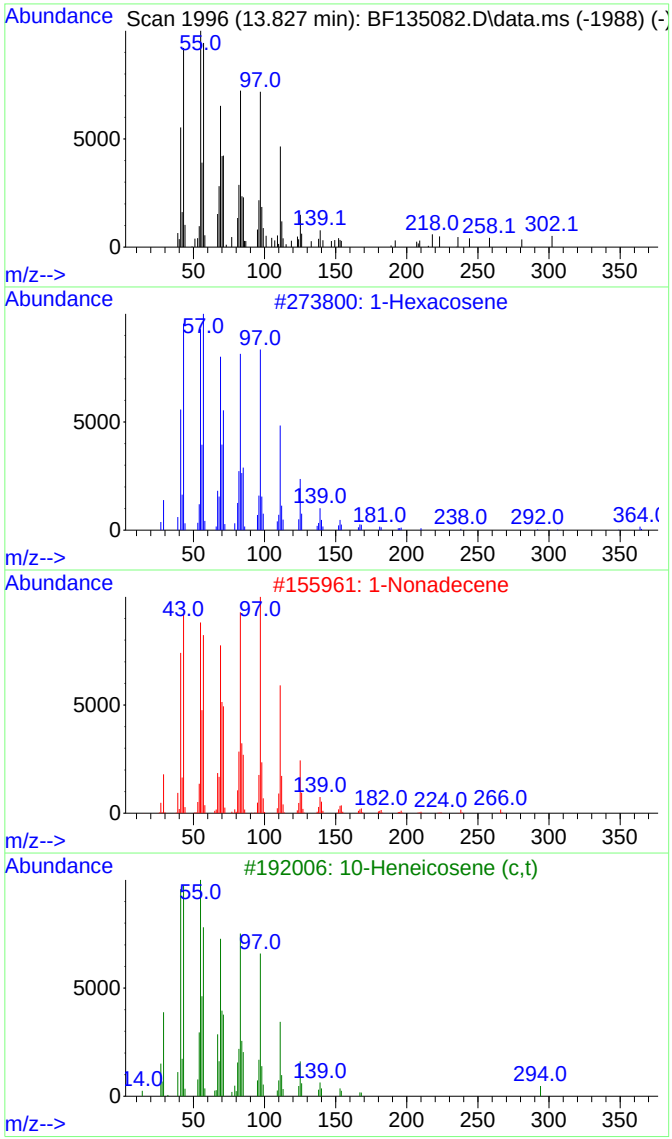
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

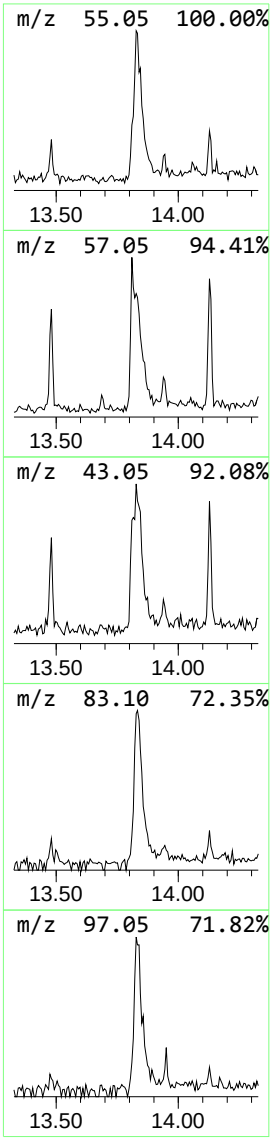
****

Peak Number 3 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.73 ng	173553	Chrysene-d12	13.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	10-Heneicosene (c,t)	294	C21H42	095008-11-0	91
4	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	90
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90





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TIC Library : C:\Database\NIST20.L
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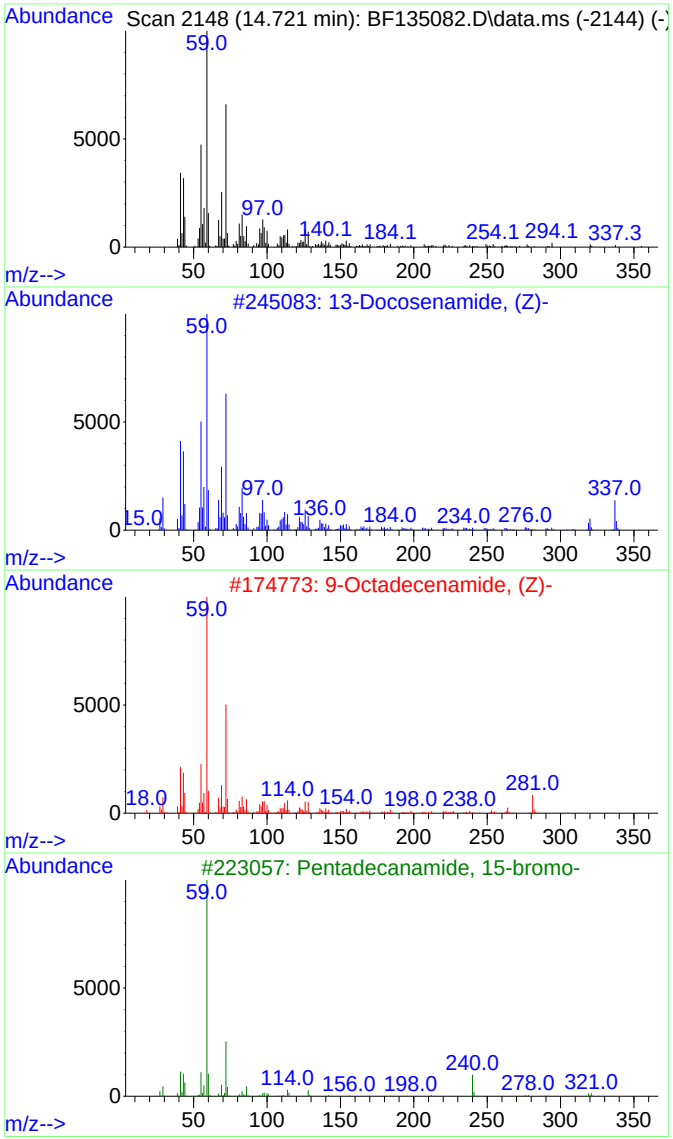
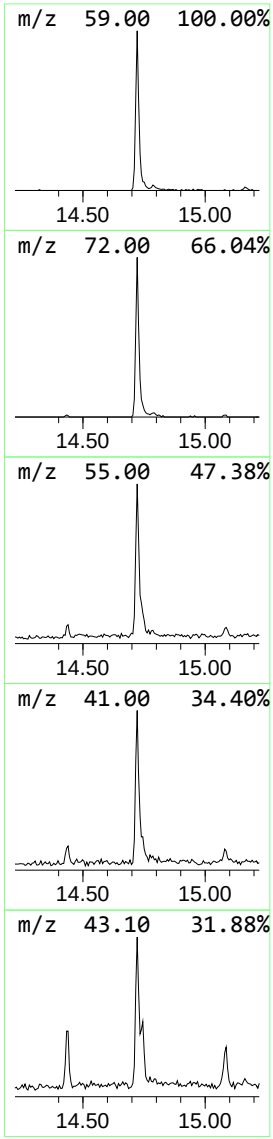
****

Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	8.65 ng	273730	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
3	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

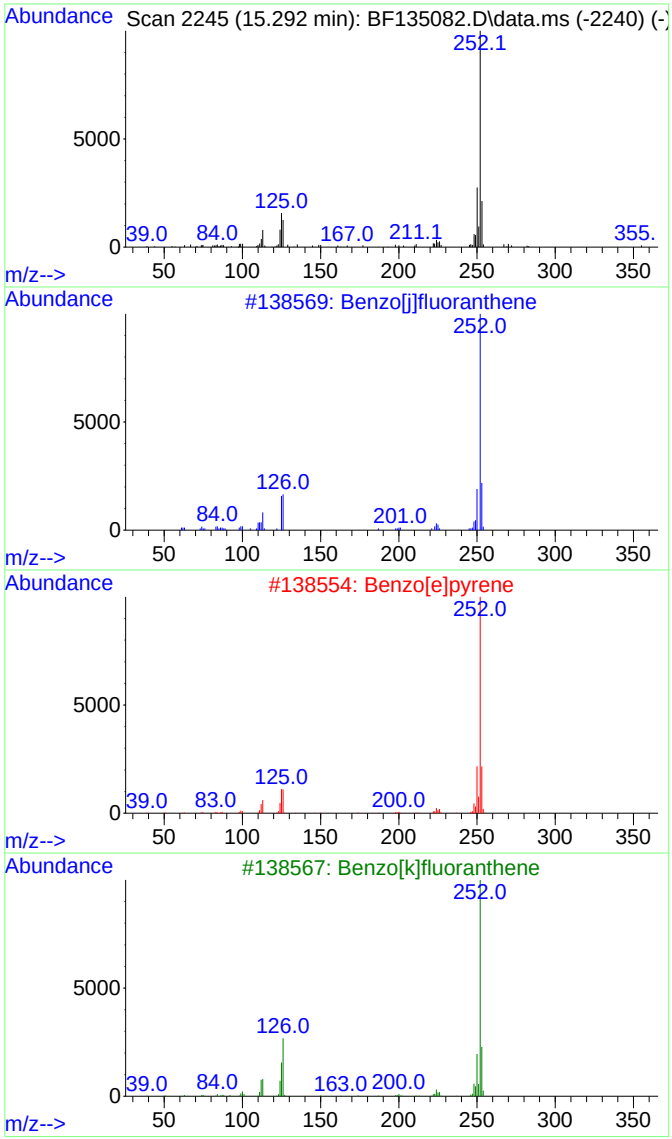
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

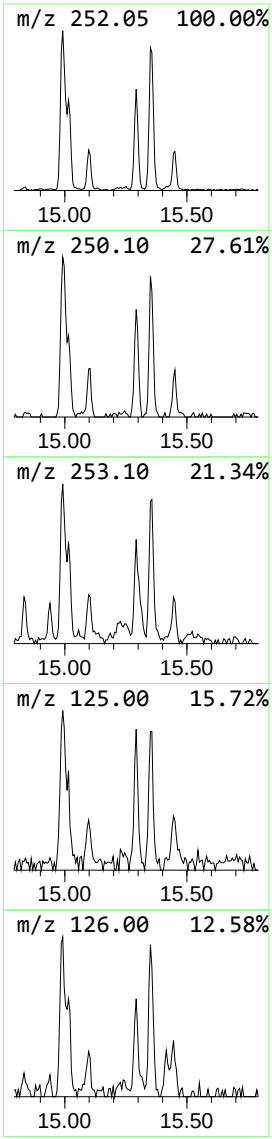
****

Peak Number 5 Benzo[j]fluoranthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	2.50 ng	79135	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





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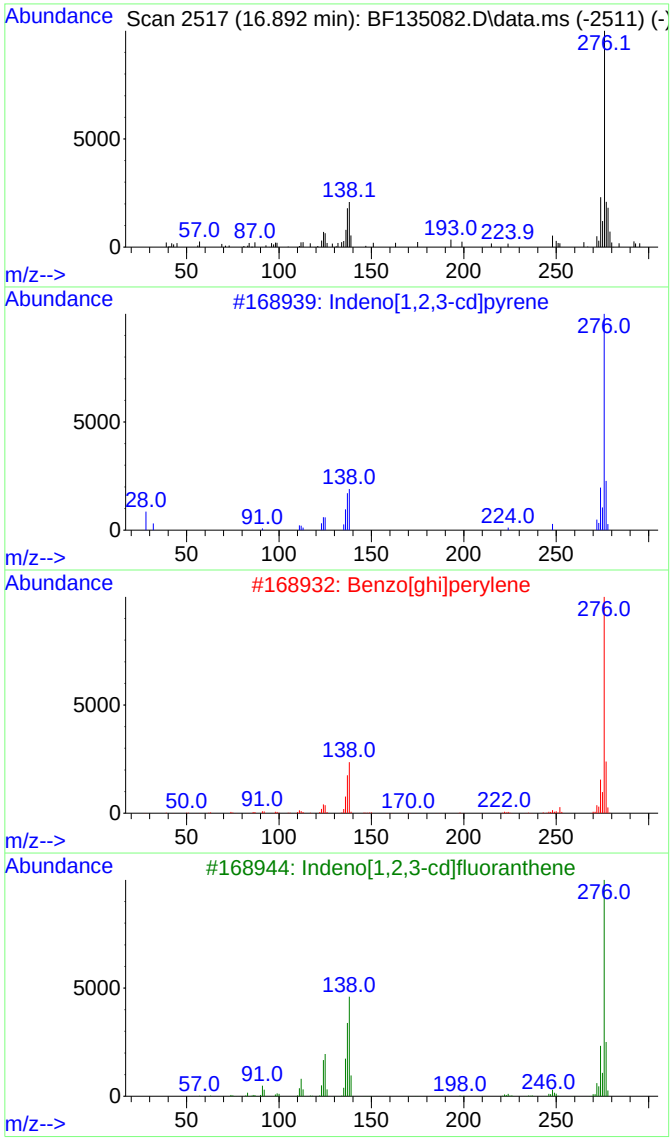
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

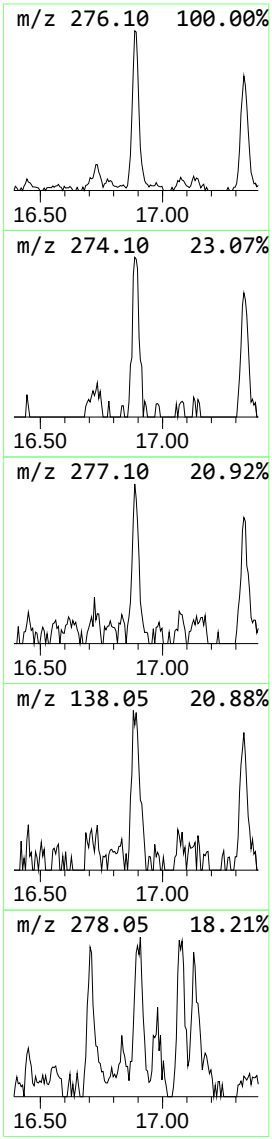
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indeno[1,2,3-cd]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.892	2.01 ng	63593	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	96
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	94
3	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	90
4	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	90
5	2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	53





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.998	2.6	ng	76890	1	6.769	595879	20.0
n-Hexadecanoic ...	11.833	5.2	ng	193322	4	11.298	738964	20.0
1-Hexacosene	13.827	4.7	ng	173553	5	13.951	734462	20.0
13-Docosenamide...	14.721	8.7	ng	273730	6	15.421	632642	20.0
Benzo[j]fluoran...	15.292	2.5	ng	79135	6	15.421	632642	20.0
Indeno[1,2,3-cd...	16.892	2.0	ng	63593	6	15.421	632642	20.0