LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136340.D
Acq On : 01 Dec 2023 16:26
Operator : CG\JU
Sample : 05366-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-13(10-15)

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136340.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	498	503	508	rVB	32422	40225	1.47%	0.225%
2	5.440	565	570	573	rBV	2215295	1987439	72.70%	11.094%
3	6.440	735	740	743	rBV	2121368	2025211	74.08%	11.305%
4	6.804	798	802	806	rBV	947962	724763	26.51%	4.046%
5	6.981	829	832	836	rVB	34567	28802	1.05%	0.161%
6	7.363	886	897	900	rBV	1537086	1371502	50.17%	7.656%
7	8.081	1014	1019	1022	rBV	1182342	1028091	37.61%	5.739%
8	8.104	1022	1023	1026	rVB	126001	59945	2.19%	0.335%
9	8.792	1138	1140	1144	rVB	40567	32430	1.19%	0.181%
10	8.892	1152	1157	1160	rVB	50579	40630	1.49%	0.227%
11	9.163	1197	1203	1206	rBV	2996262	2733691	100.00%	15.260%
12	9.428	1242	1248	1251	rBV4	19401	28899	1.06%	0.161%
13	9.498	1257	1260	1262	rBV	31313	29723	1.09%	0.166%
14	9.698	1289	1294	1298	rVB	257534	208818	7.64%	1.166%
15	9.839	1311	1318	1321	rBV	1382907	1118927	40.93%	6.246%
16	9.869	1321	1323	1329	rVB	56264	55876	2.04%	0.312%
17	10.386	1408	1411	1413	rBV	40306	36464	1.33%	0.204%
18	10.498	1424	1430	1433	rBV	42409	47388	1.73%	0.265%
19	10.628	1448	1452	1466	rBV	1271186	1173866	42.94%	6.553%
20	10.763	1471	1475	1481	rVB	81481	100326	3.67%	0.560%
21	11.227	1551	1554	1558	rVB2	78991	93174	3.41%	0.520%
22	11.327	1568	1571	1574	rBV	1007636	890892	32.59%	4.973%
23	11.351	1574	1575	1580	rVV	197782	134212	4.91%	0.749%
24	11.404	1581	1584	1586	rVB	47588	44182	1.62%	0.247%
25	11.663	1625	1628	1636	rVB2	31157	37966	1.39%	0.212%
26	11.863	1659	1662	1666	rBV2	109762	97411	3.56%	0.544%
27	11.945	1673	1676	1678	rBV	51170	55970	2.05%	0.312%
28	12.322	1736	1740	1746	rVB5	26620	43526	1.59%	0.243%
29	12.386	1748	1751	1754	rBV2	41609	39983	1.46%	0.223%
30	12.463	1762	1764	1770	rVB	27720	35859	1.31%	0.200%
31	12.545	1774	1778	1783	rBV	89337	94842	3.47%	0.529%
32	12.651	1792	1796	1802	rBV3	22205	39739	1.45%	0.222%
33	12.774	1814	1817	1820	rVB	108959	83576	3.06%	0.467%
34	12.927	1839	1843	1846	rBV	1901193	1627560	59.54%	9.085%
35	13.104	1871	1873	1877	rVB2	24083	28643	1.05%	0.160%
36	13.839	1995	1998	2003	rVB3	27388	32569	1.19%	0.182%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P-13(10-15)

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.980	2017	2022	2025	rBV	613238	614747	22.49%	3.432%
38	14.757	2150	2154	2166	rBV2	131902	192048	7.03%	1.072%
39	15.033	2197	2201	2210	rVB3	28180	62371	2.28%	0.348%
40	15.127	2214	2217	2223	rVB4	26469	36434	1.33%	0.203%
41	15.398	2259	2263	2267	rBV2	27656	37320	1.37%	0.208%
42	15.463	2269	2274	2281	rVV	499450	635856	23.26%	3.550%
43	15.515	2281	2283	2292	rVB6	20820	44500	1.63%	0.248%
44	16.915	2516	2521	2525	rBV2	23409	37554	1.37%	0.210%

Sum of corrected areas: 17913950

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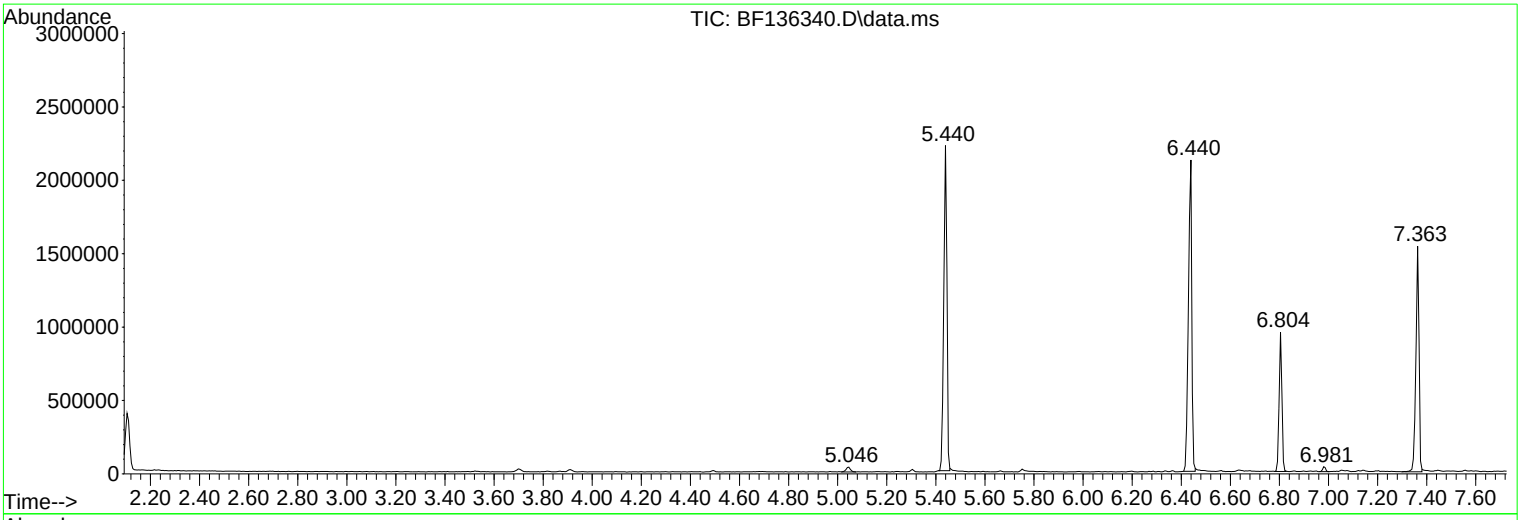
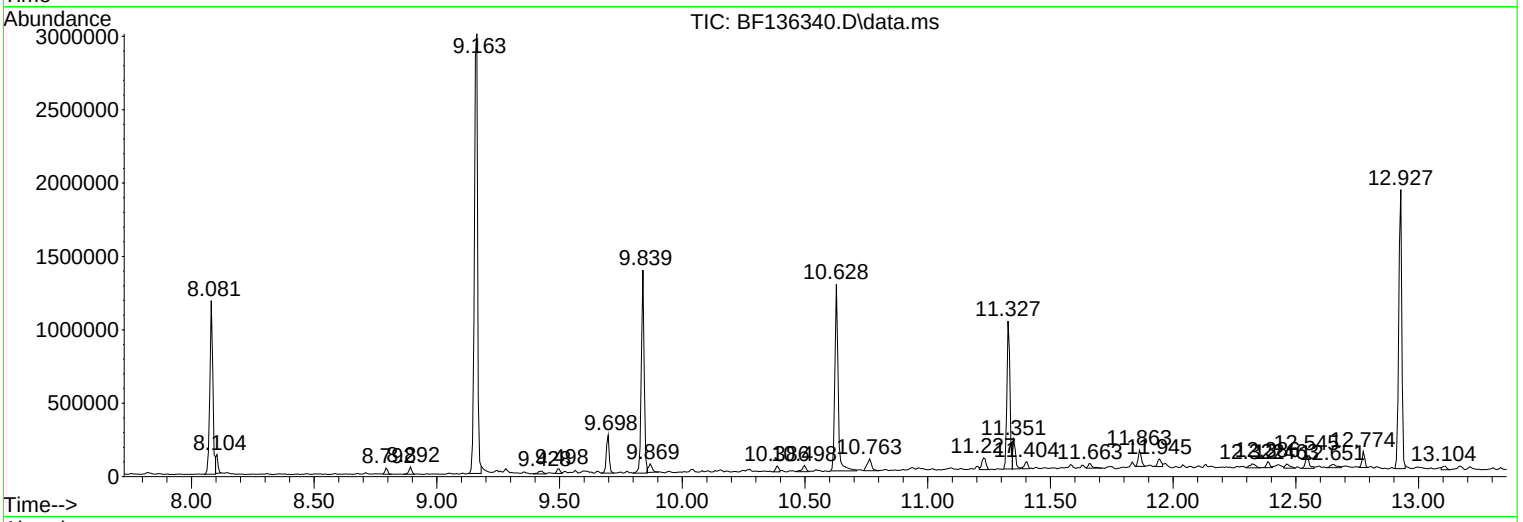
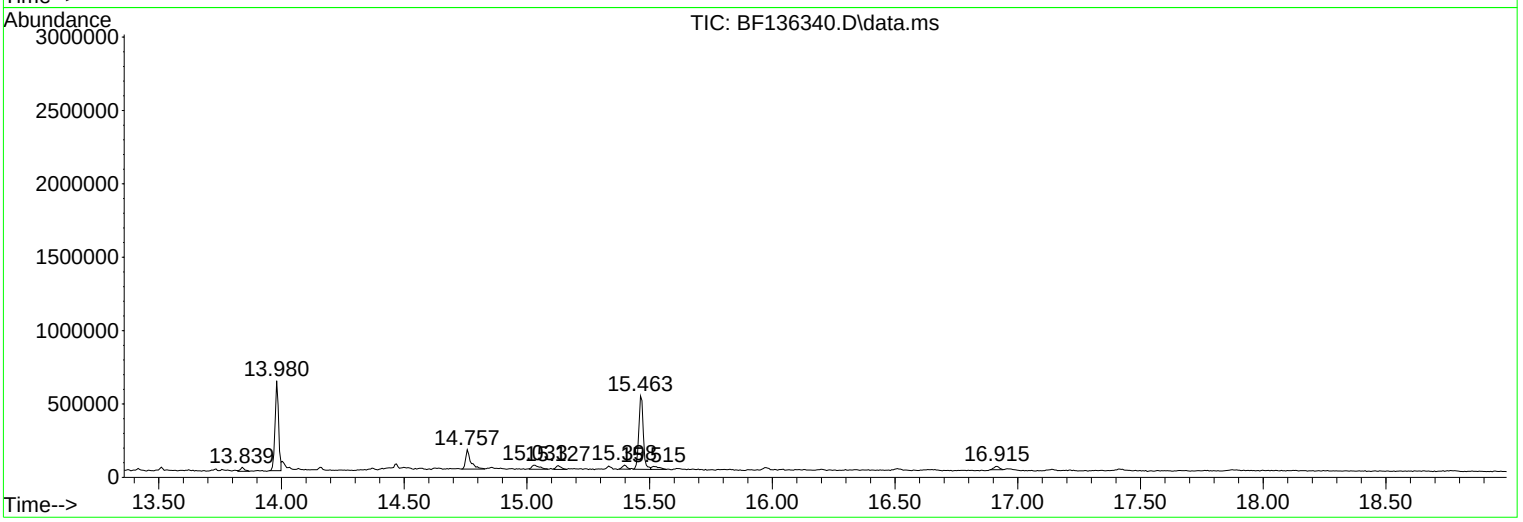
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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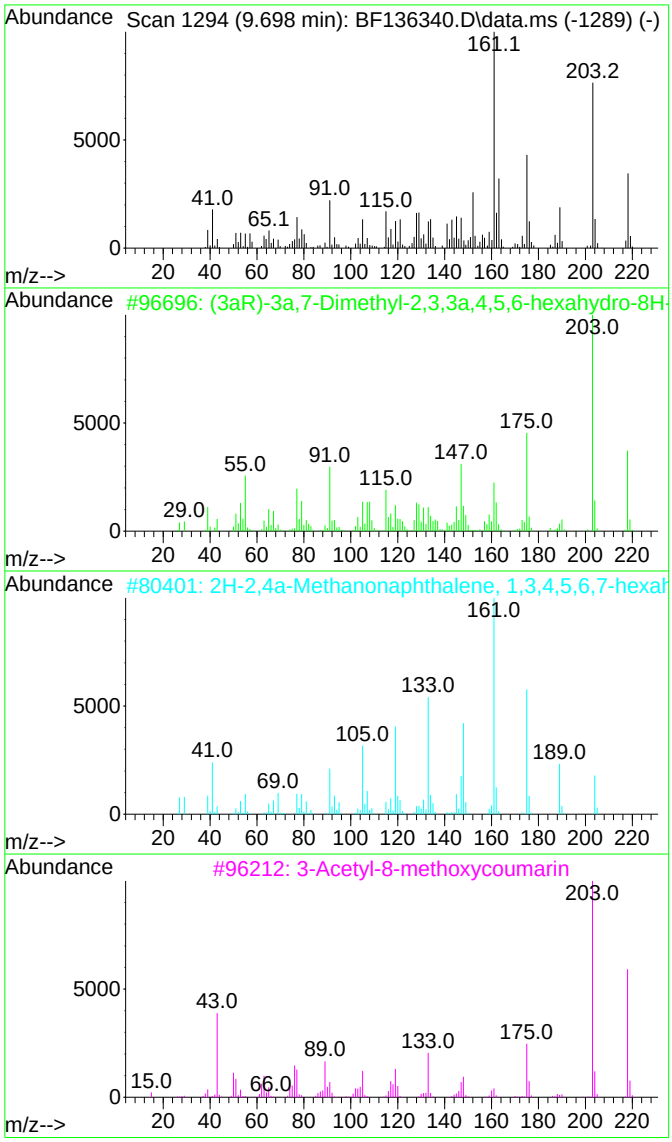
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

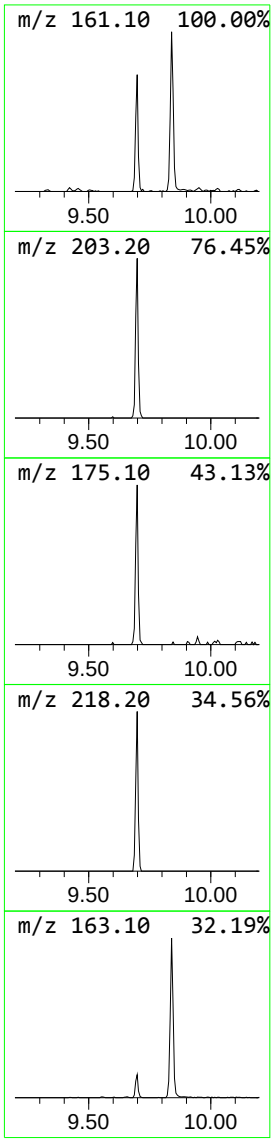
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (3aR)-3a,7-Dimethyl-2,3,3a,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.698	3.73 ng	208818	Acenaphthene-d10	9.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3aR)-3a,7-Dimethyl-2,3,3a,4,5,6...	218	C14H18O2	1000482-61-7	70
2	2H-2,4a-Methanonaphthalene, 1,3,...	204	C15H24	001135-66-6	64
3	3-Acetyl-8-methoxycoumarin	218	C12H10O4	005452-39-1	38
4	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	38
5	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	38





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Sample : 05366-01
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-13(10-15)

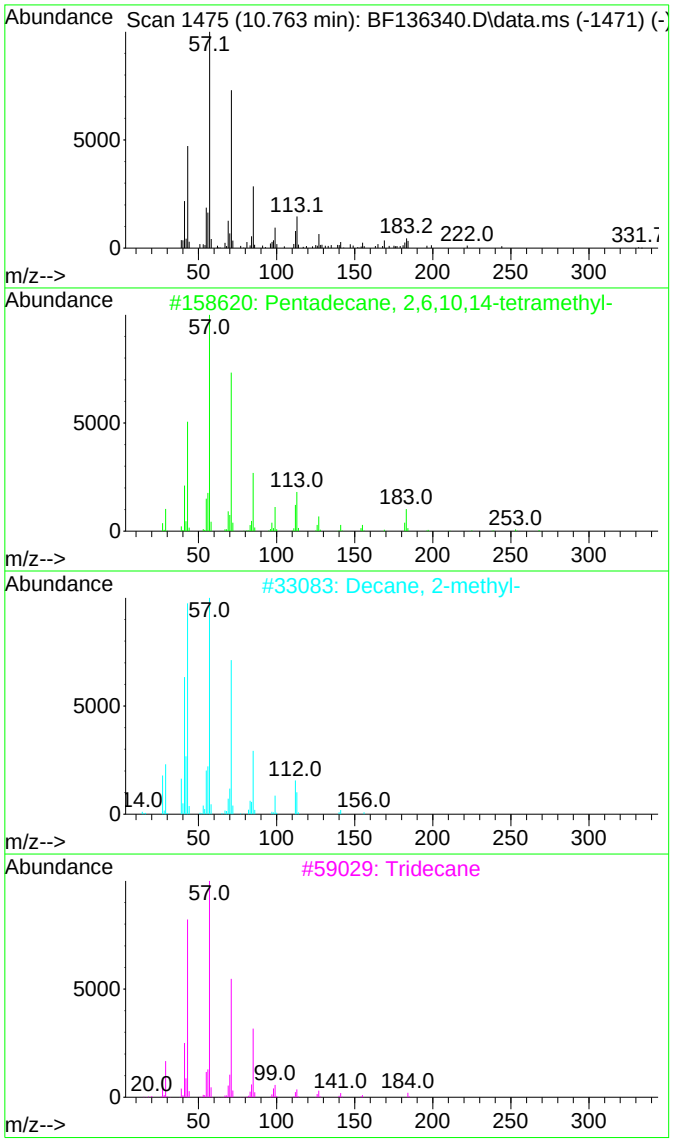
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

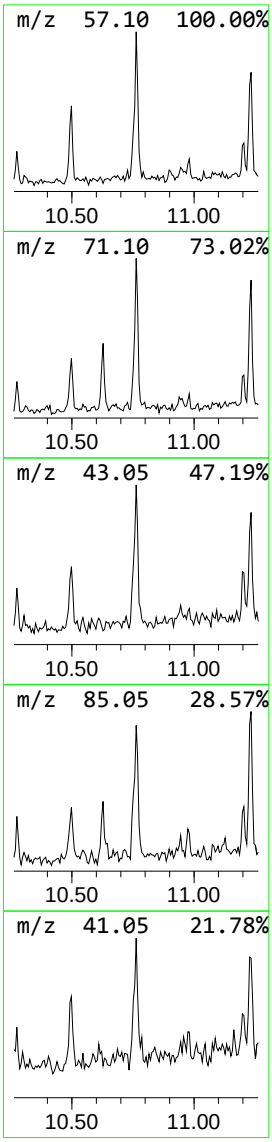
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentadecane, 2,6,10,14-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.763	2.25 ng	100326	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	87
2	Decane, 2-methyl-	156	C11H24	006975-98-0	80
3	Tridecane	184	C13H28	000629-50-5	72
4	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	64
5	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64





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Operator : CG\JU
Sample : 05366-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
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P-13(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

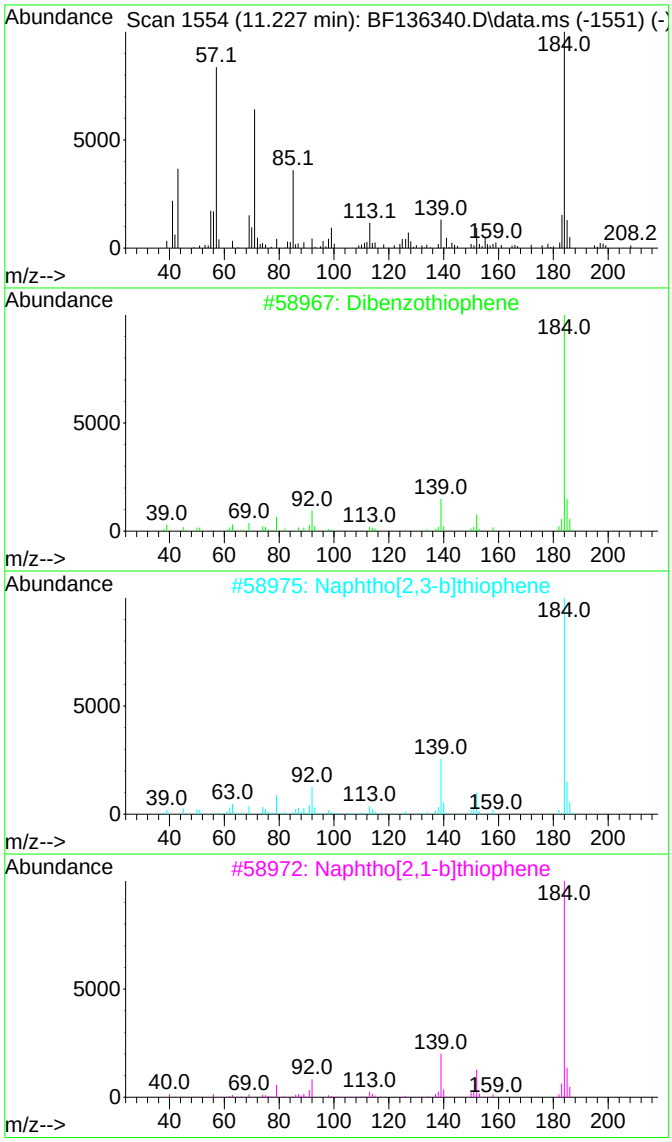
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

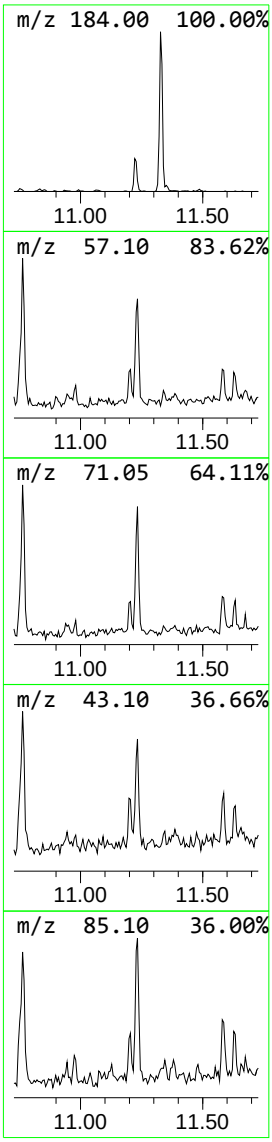
****

Peak Number 3 Dibenzothiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.227	2.09 ng	93174	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	60
2	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	49
3	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	49
4	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	46
5	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	43





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P-13(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

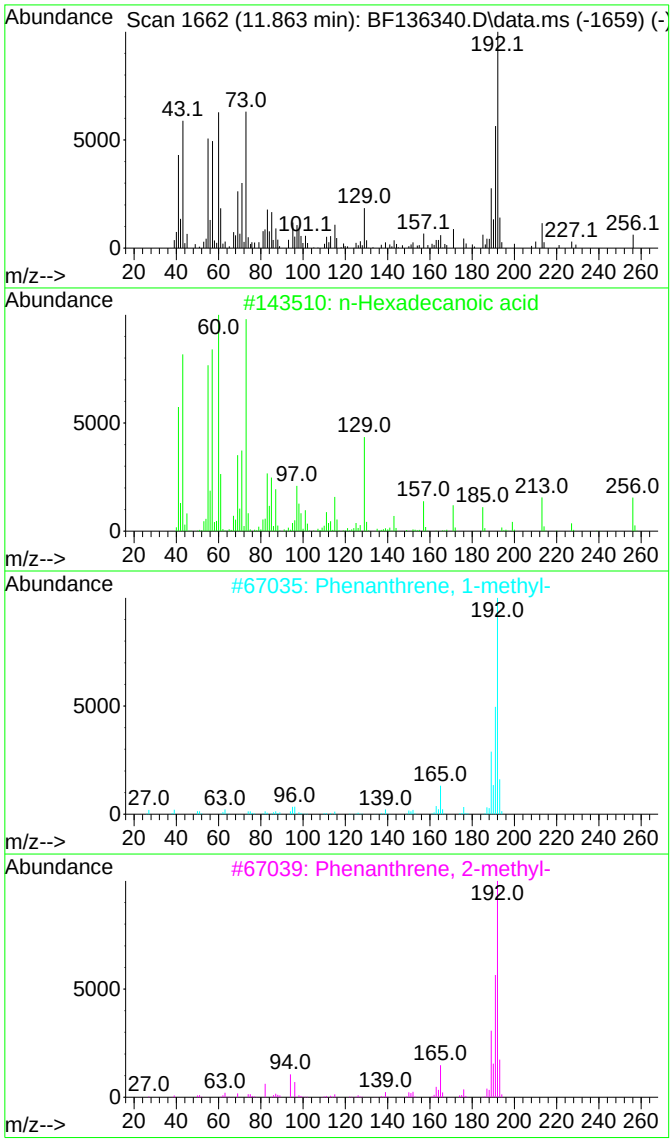
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

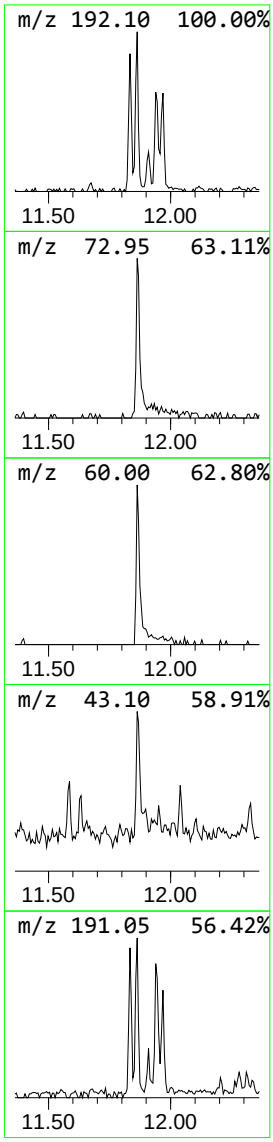
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	2.19 ng	97411	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	78
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	70





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P-13(10-15)

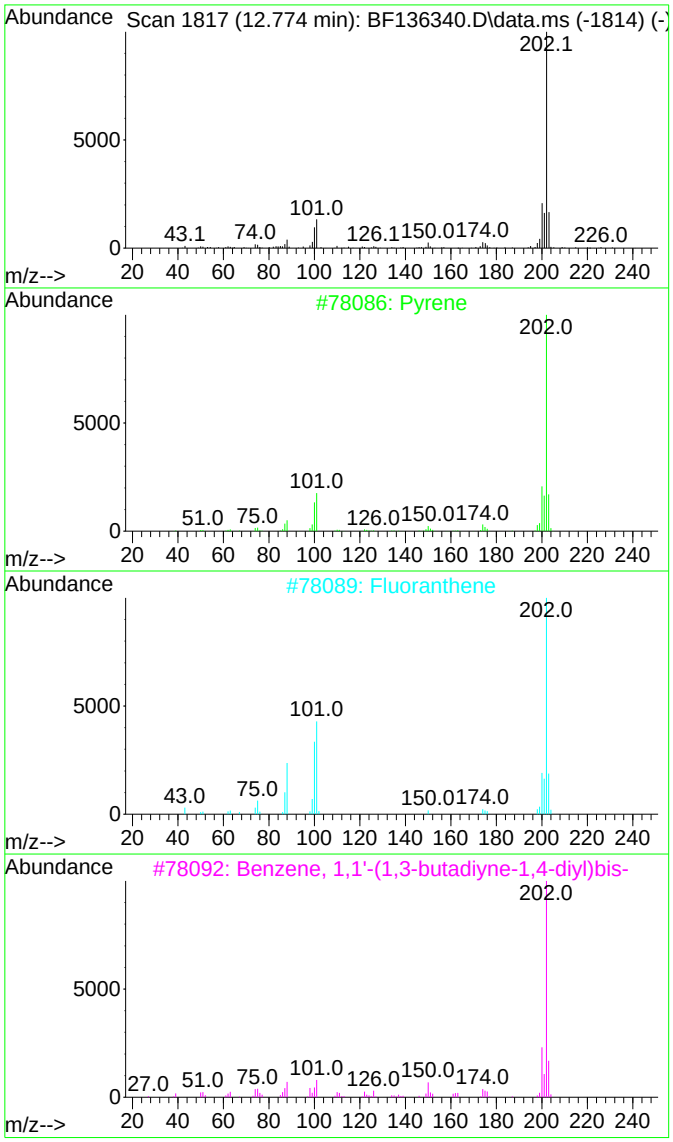
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

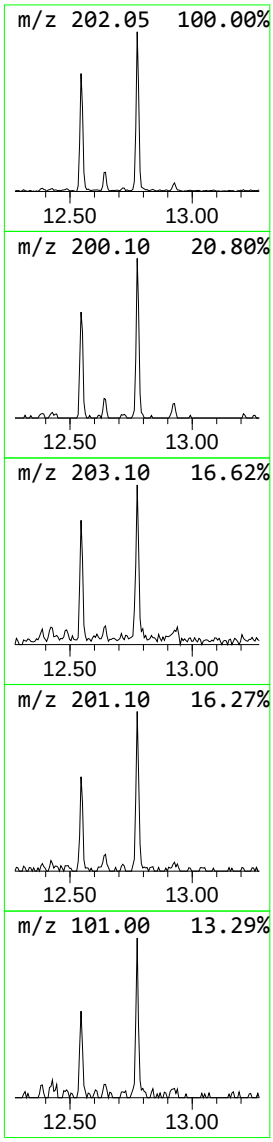
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.775	2.72 ng	83576	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	94
2	Fluoranthene	202	C16H10	000206-44-0	87
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
4	l-Leucine, N-methyl-N-(2-methoxy...	485	C28H55NO5	1010328-55-1	40
5	l-Leucine, N-methyl-N-(2-methoxy...	359	C19H37NO5	1000328-54-3	40





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ALS Vial : 13 Sample Multiplier: 1

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BNA_F
ClientSampleId :
P-13(10-15)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

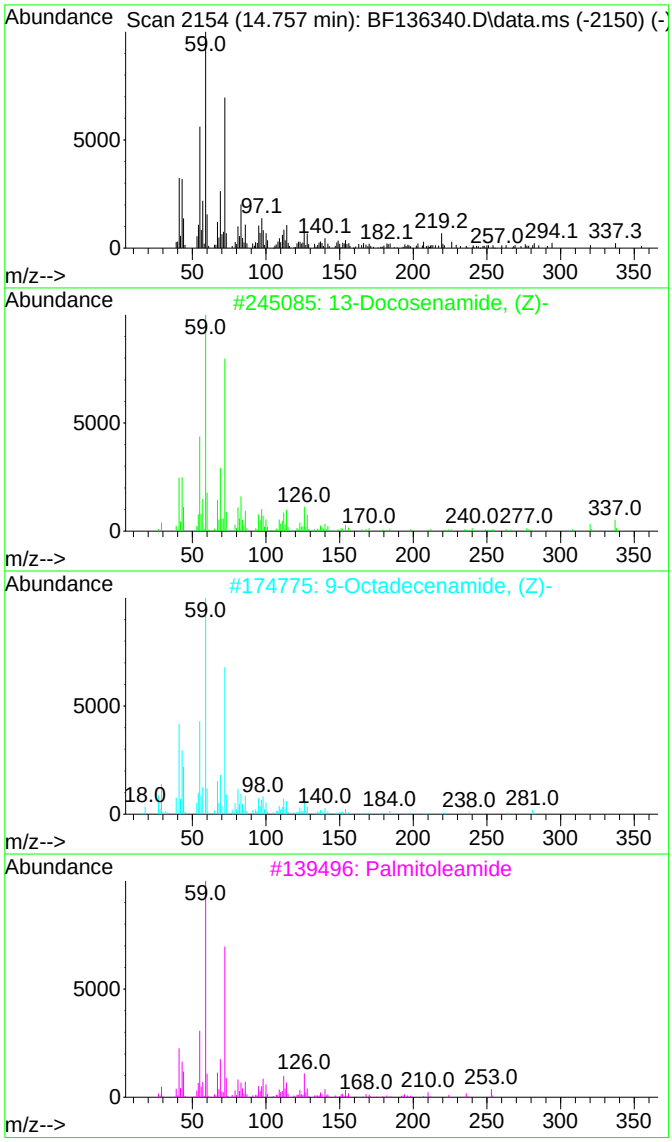
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

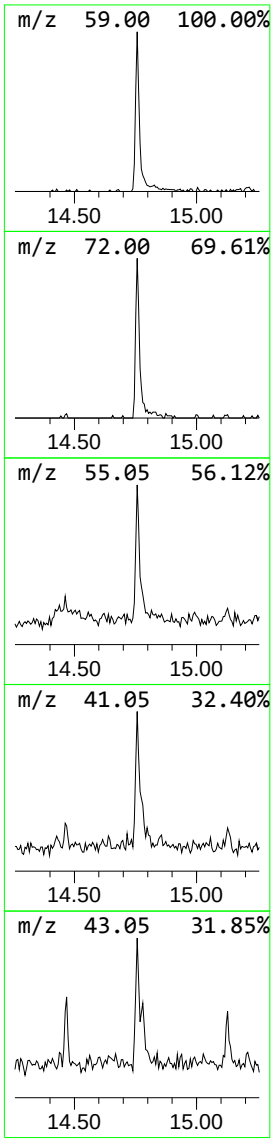
****

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	6.04 ng	192048	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	96
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
3	Palmitoleamide	253	C16H31NO	106010-22-4	53
4	7-Nonenamide	155	C9H17NO	090949-53-4	53
5	Nonanamide	157	C9H19NO	001120-07-6	47





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
(3aR)-3a,7-Dime...	9.698	3.7	ng	208818	3	9.839	1118930	20.0
Pentadecane, 2,...	10.763	2.3	ng	100326	4	11.328	890892	20.0
Dibenzothiophene	11.227	2.1	ng	93174	4	11.328	890892	20.0
n-Hexadecanoic ...	11.863	2.2	ng	97411	4	11.328	890892	20.0
Benzene, 1,1'-(...	12.775	2.7	ng	83576	5	13.980	614747	20.0
13-Docosenamide...	14.757	6.0	ng	192048	6	15.463	635856	20.0