LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128683.D
Acq On : 03 Jun 2022 17:09
Operator : CG\JU
Sample : N3113-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
357

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128683.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	463	466	475	rVB	141119	165856	8.82%	1.152%
2	5.469	537	541	550	rBV	1655728	1683294	89.56%	11.689%
3	6.481	710	713	724	rBV	1820079	1717806	91.40%	11.928%
4	6.563	724	727	730	rVB	32898	22197	1.18%	0.154%
5	6.822	767	771	774	rBV	644020	496479	26.42%	3.448%
6	7.387	861	867	870	rBV	1325684	1170345	62.27%	8.127%
7	8.104	985	989	993	rBV	738705	595705	31.69%	4.137%
8	9.181	1167	1172	1176	rBV	2138362	1879501	100.00%	13.051%
9	9.863	1284	1288	1291	rBV	676912	562330	29.92%	3.905%
10	10.651	1418	1422	1426	rBV	1160816	952225	50.66%	6.612%
11	11.345	1537	1540	1543	rBV	538277	503130	26.77%	3.494%
12	11.369	1543	1544	1548	rVV	120956	84251	4.48%	0.585%
13	11.422	1548	1553	1556	rVB	30319	26720	1.42%	0.186%
14	11.580	1574	1580	1585	rBV2	13243	24978	1.33%	0.173%
15	11.851	1623	1626	1628	rBV	31788	26437	1.41%	0.184%
16	11.880	1628	1631	1636	rVV	107755	96099	5.11%	0.667%
17	11.963	1641	1645	1647	rBV2	38621	39031	2.08%	0.271%
18	12.398	1716	1719	1722	rBV	28352	27075	1.44%	0.188%
19	12.486	1731	1734	1739	rBV5	18490	23454	1.25%	0.163%
20	12.563	1743	1747	1752	rVB	218329	190540	10.14%	1.323%
21	12.663	1761	1764	1767	rBV3	29990	31491	1.68%	0.219%
22	12.792	1780	1786	1789	rBV	192517	204997	10.91%	1.423%
23	12.939	1807	1811	1814	rBV	1793699	1530211	81.42%	10.626%
24	13.010	1819	1823	1826	rBV4	19895	28108	1.50%	0.195%
25	13.116	1839	1841	1844	rVB	30683	32303	1.72%	0.224%
26	13.186	1847	1853	1856	rBV2	30027	43851	2.33%	0.304%
27	13.221	1856	1859	1862	rVB	32981	30592	1.63%	0.212%
28	13.627	1925	1928	1933	rVB	24929	30986	1.65%	0.215%
29	13.739	1943	1947	1950	rBV3	19322	28058	1.49%	0.195%
30	13.868	1961	1969	1982	rBV6	45995	180537	9.61%	1.254%
31	13.992	1984	1990	1993	rBV2	618171	674342	35.88%	4.683%
32	14.015	1993	1994	2001	rVB	127314	85714	4.56%	0.595%
33	14.086	2002	2006	2012	rBV	233454	259342	13.80%	1.801%
34	15.027	2162	2166	2169	rBV	100327	142370	7.57%	0.989%
35	15.110	2177	2180	2183	rBV	32697	35421	1.88%	0.246%
36	15.327	2214	2217	2223	rVB	53154	69801	3.71%	0.485%

LSC Area Percent Report

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Data File : BF128683.D
Acq On : 03 Jun 2022 17:09
Operator : CG\JU
Sample : N3113-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
357

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.392	2224	2228	2234	rBV	83042	100310	5.34%	0.697%
38	15.457	2234	2239	2243	rBV	365618	438897	23.35%	3.048%
39	15.927	2316	2319	2324	rBV3	33975	45318	2.41%	0.315%
40	16.433	2401	2405	2411	rVB5	17320	35717	1.90%	0.248%
41	17.339	2554	2559	2569	rVB	32172	85170	4.53%	0.591%

Sum of corrected areas: 14400989

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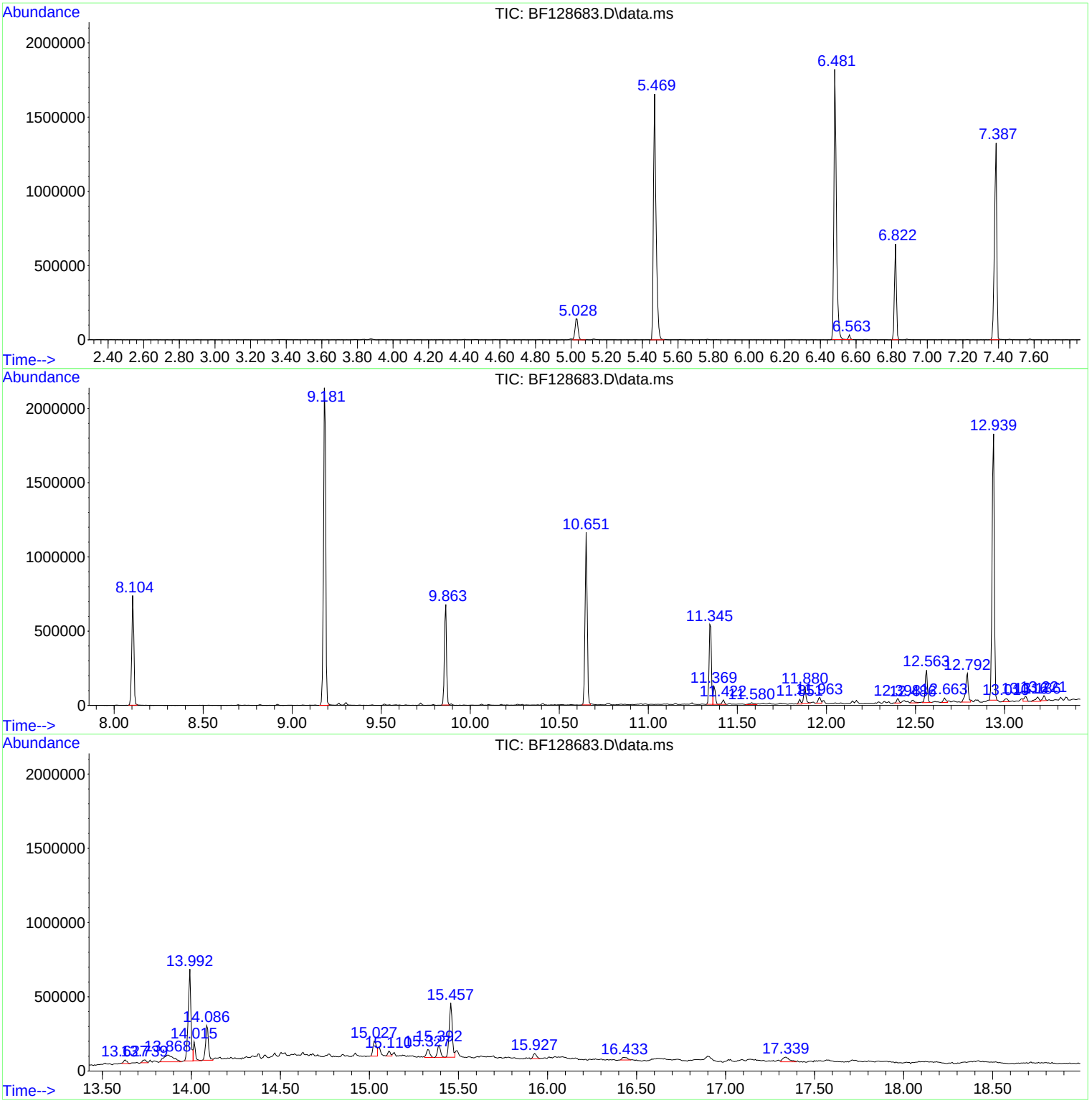
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF128683.D
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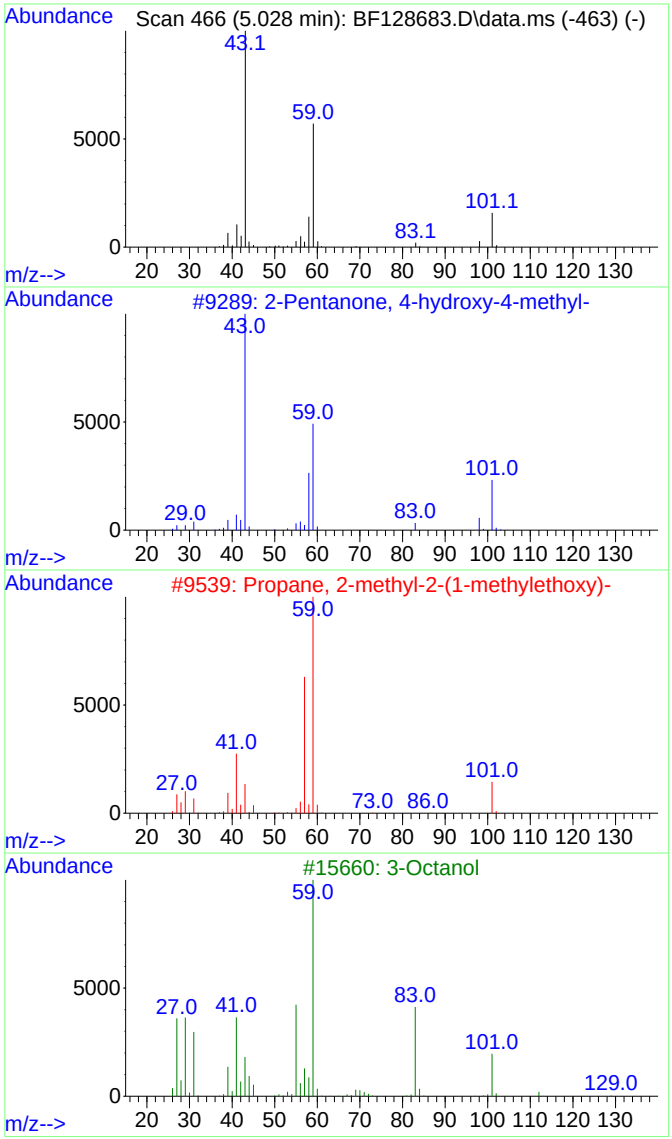
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

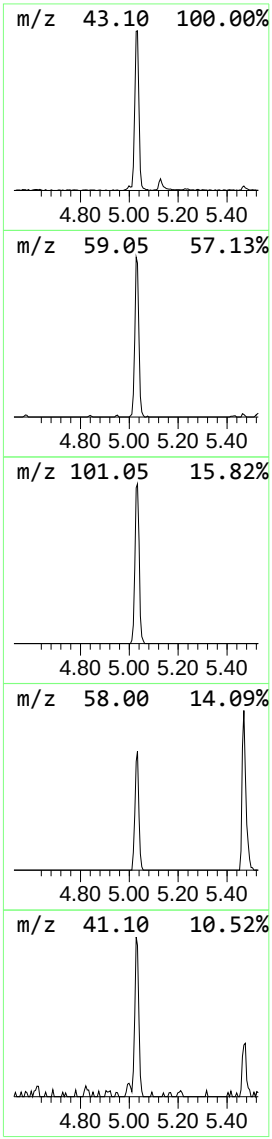
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	6.68 ng	165856	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Octanol	130	C8H18O	000589-98-0	33
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





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Instrument :
BNA_F
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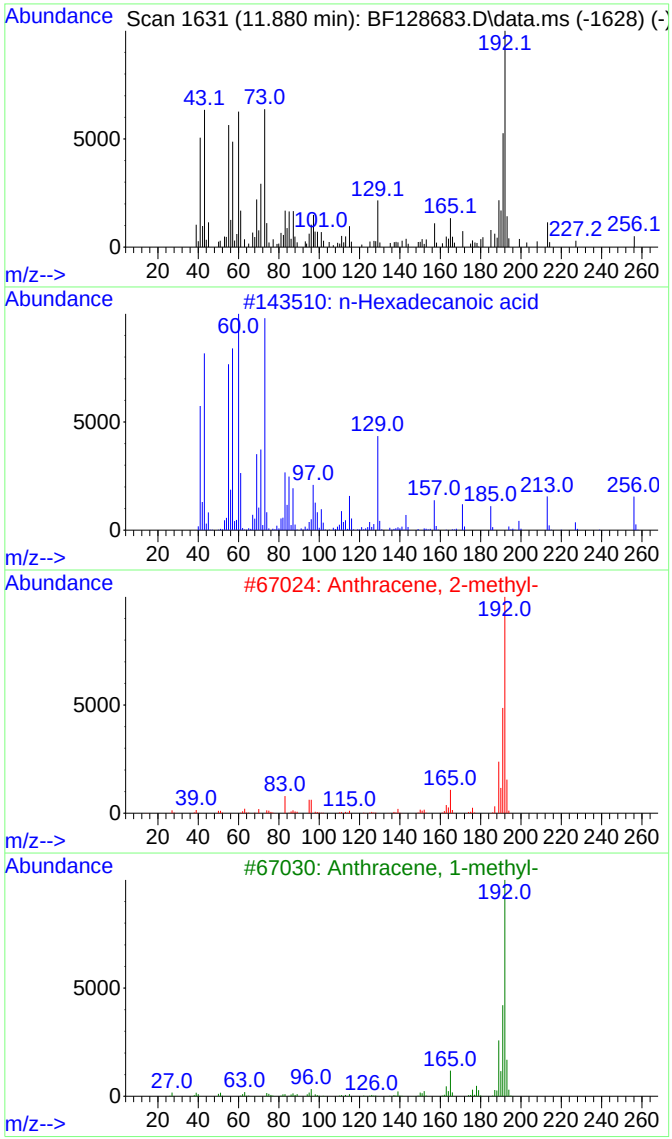
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

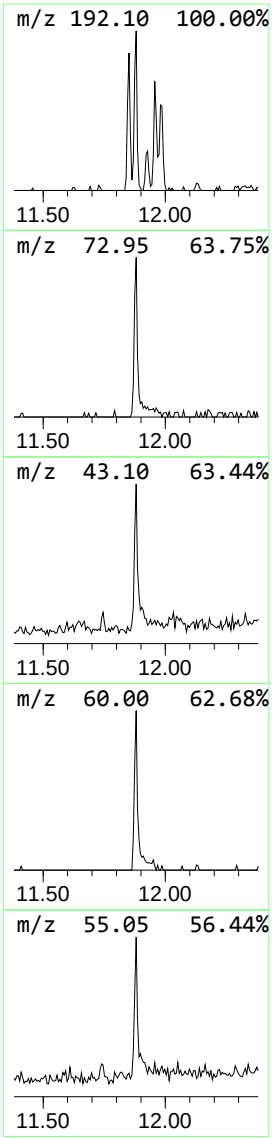
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	3.82 ng	96099	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	70
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	60





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

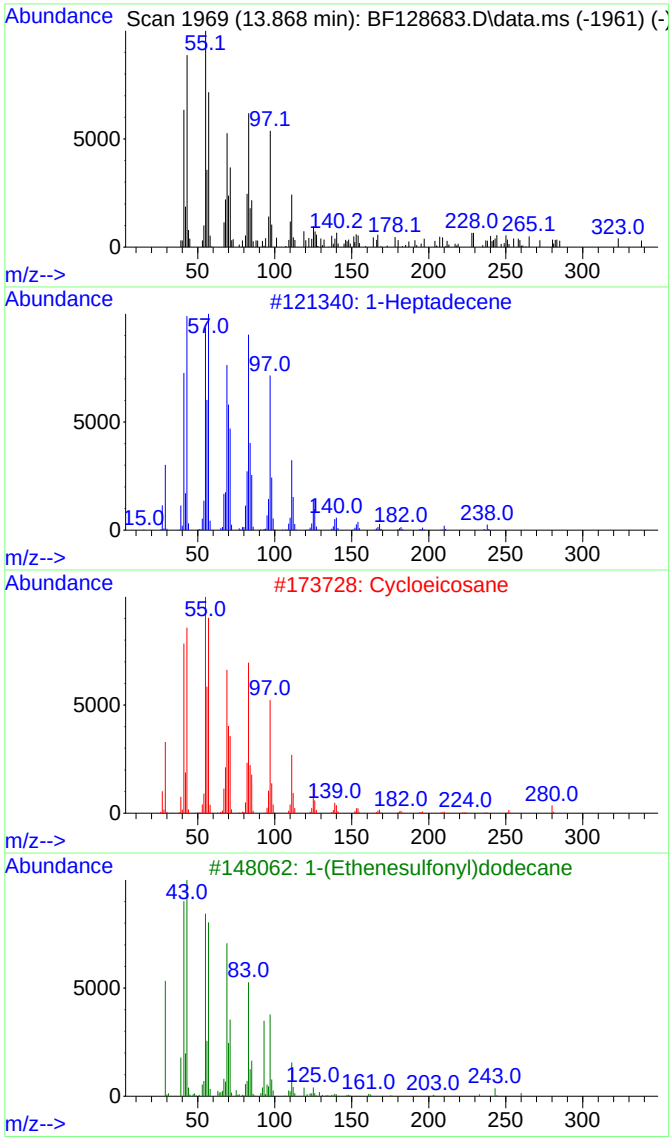
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

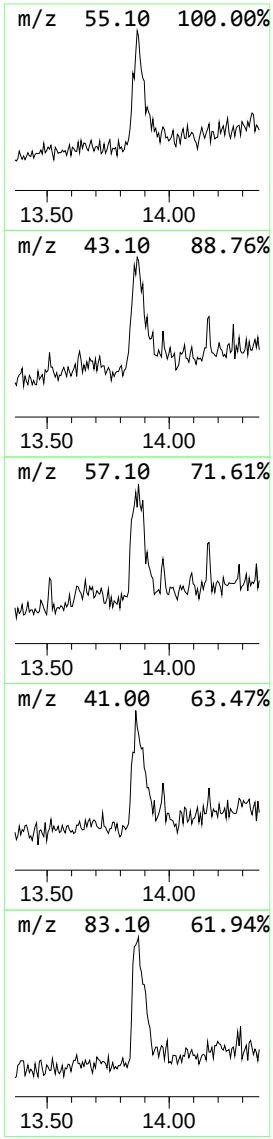
****

Peak Number 3 1-Heptadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	5.35 ng	180537	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	90
2	Cycloeicosane	280	C20H40	000296-56-0	89
3	1-(Ethenesulfonyl)dodecane	260	C14H28O2S	030719-66-5	86
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
5	1-Tricosene	322	C23H46	018835-32-0	74





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Sample : N3113-01
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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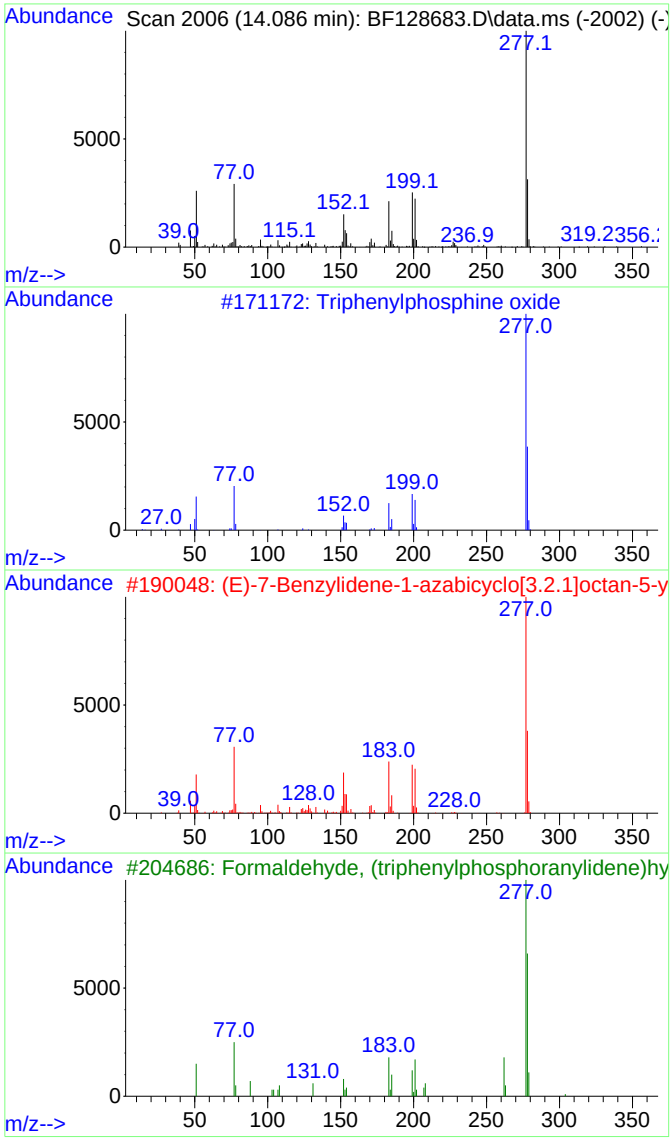
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

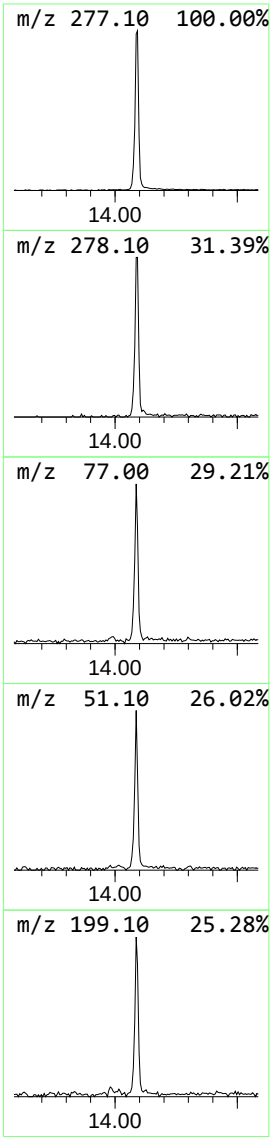
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	7.69 ng	259342	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	80
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	39
5	Dimethoxymethyl-hydroxy-tripheny...	354	C21H23O3P	1000132-00-1	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

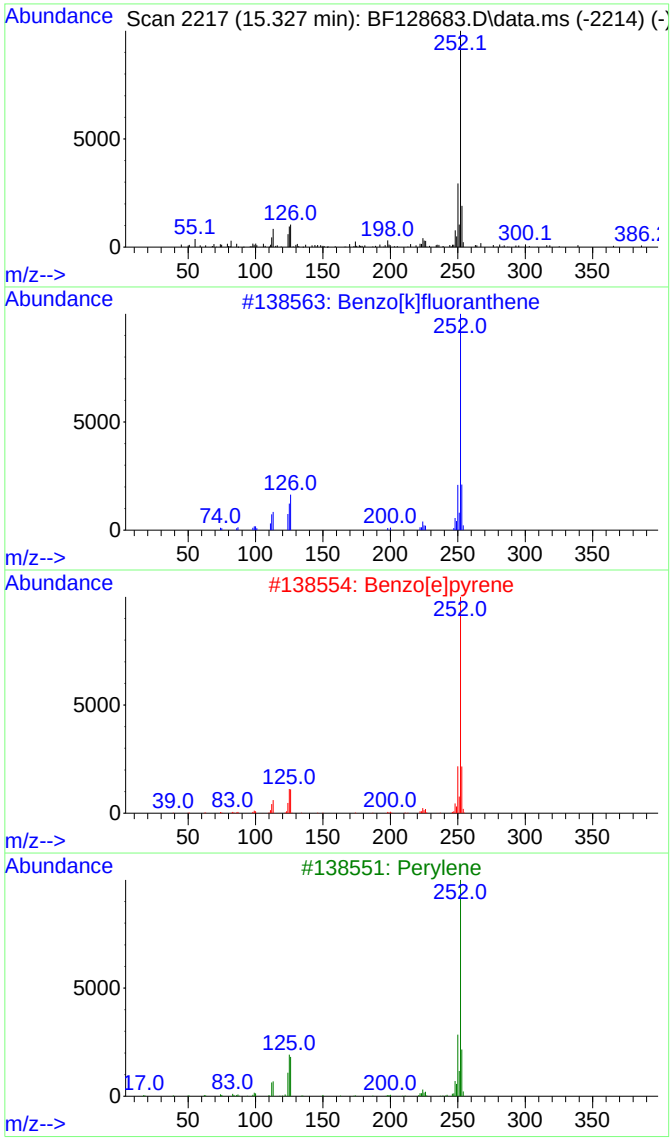
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

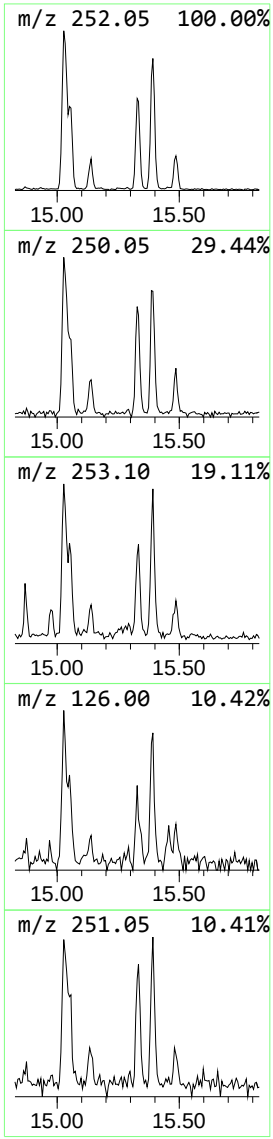
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	3.18 ng	69801	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
2	Benzo[e]pyrene	252	C20H12	000192-97-2	97
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

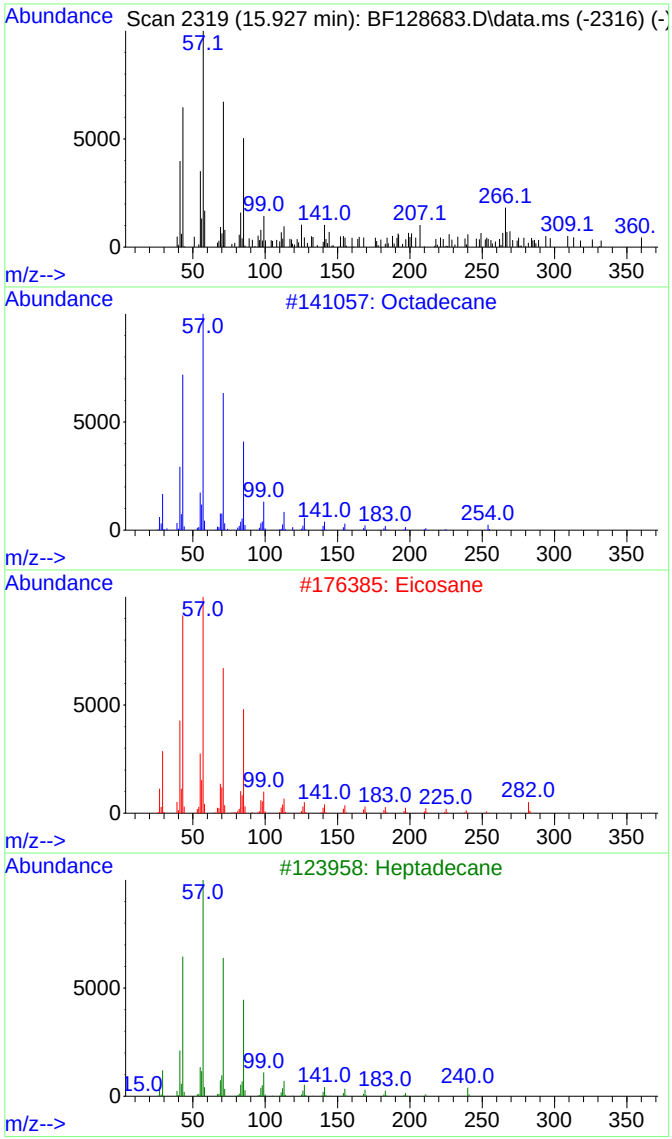
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

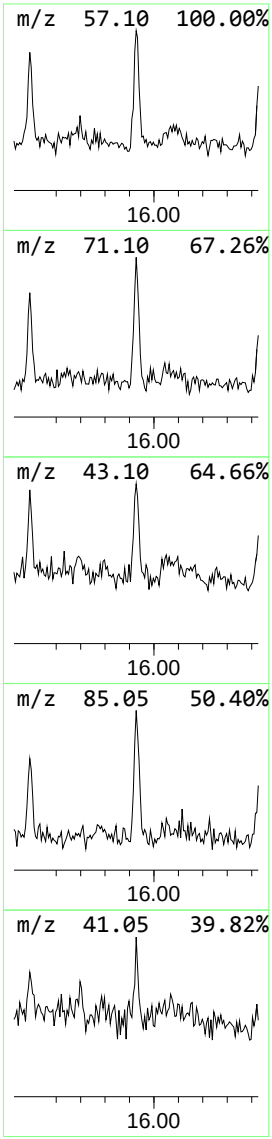
****

Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	2.07 ng	45318	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	83
2	Eicosane	282	C20H42	000112-95-8	78
3	Heptadecane	240	C17H36	000629-78-7	60
4	9-Methylheneicosane	310	C22H46	070475-51-3	49
5	Triacontane	422	C30H62	000638-68-6	49





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-...	5.028	6.7	ng	165856	1	6.822	496479	20.0
n-Hexadecanoic ...	11.880	3.8	ng	96099	4	11.351	503130	20.0
1-Heptadecene	13.868	5.3	ng	180537	5	13.992	674342	20.0
Triphenylphosph...	14.086	7.7	ng	259342	5	13.992	674342	20.0
Benzo[e]pyrene	15.327	3.2	ng	69801	6	15.457	438897	20.0
Octadecane	15.927	2.1	ng	45318	6	15.457	438897	20.0