LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072023\
Data File : BF134388.D
Acq On : 20 Jul 2023 18:47
Operator : CG\JU
Sample : 03654-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12016

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134388.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	3	14	21	rVB	174349	260618	10.37%	1.453%
2	5.481	573	577	580	rBV	1884808	1716162	68.31%	9.569%
3	6.481	742	747	750	rBV	1870697	1769543	70.43%	9.867%
4	6.834	804	807	818	rBV	458686	393484	15.66%	2.194%
5	7.404	899	904	907	rBV	1239957	1159248	46.14%	6.464%
6	8.116	1021	1025	1037	rBV	592434	524201	20.86%	2.923%
7	9.192	1204	1208	1211	rBV	2917229	2295809	91.38%	12.801%
8	9.498	1257	1260	1263	rBV	59769	48249	1.92%	0.269%
9	9.586	1271	1275	1279	rVB2	65683	61008	2.43%	0.340%
10	9.869	1320	1323	1327	rBV	655814	590882	23.52%	3.295%
11	10.669	1455	1459	1462	rBV	1513601	1352518	53.83%	7.542%
12	11.369	1574	1578	1580	rBV	740941	663094	26.39%	3.697%
13	11.392	1580	1582	1585	rVV	387613	307821	12.25%	1.716%
14	11.439	1588	1590	1594	rVB	63125	58069	2.31%	0.324%
15	11.869	1660	1663	1666	rBV	33416	32569	1.30%	0.182%
16	11.898	1666	1668	1672	rVB	63220	54675	2.18%	0.305%
17	11.986	1679	1683	1685	rBV	67515	71734	2.86%	0.400%
18	12.198	1717	1719	1725	rVB	43425	40623	1.62%	0.227%
19	12.463	1760	1764	1770	rVB6	21127	28223	1.12%	0.157%
20	12.586	1781	1785	1789	rBV	618729	557435	22.19%	3.108%
21	12.821	1819	1825	1830	rVB	498406	530016	21.10%	2.955%
22	12.968	1842	1850	1853	rBV	2675800	2512441	100.00%	14.009%
23	13.033	1859	1861	1866	rVB2	22237	36309	1.45%	0.202%
24	13.151	1878	1881	1885	rVB	58518	60552	2.41%	0.338%
25	13.215	1890	1892	1895	rBV	46284	40310	1.60%	0.225%
26	13.257	1895	1899	1901	rBV2	34473	38728	1.54%	0.216%
27	13.380	1917	1920	1926	rBV5	17741	30961	1.23%	0.173%
28	13.774	1984	1987	1990	rBV	46243	49958	1.99%	0.279%
29	13.804	1990	1992	1994	rVB	38058	32271	1.28%	0.180%
30	13.910	2007	2010	2013	rBV4	25606	41976	1.67%	0.234%
31	14.027	2022	2030	2033	rBV2	542753	714450	28.44%	3.984%
32	14.057	2033	2035	2042	rVB	197067	176130	7.01%	0.982%
33	14.133	2042	2048	2051	rBV	46510	46152	1.84%	0.257%
34	14.568	2120	2122	2125	rBV3	22151	27922	1.11%	0.156%
35	14.674	2135	2140	2142	rBV6	24110	45864	1.83%	0.256%
36	14.792	2156	2160	2166	rVB3	47853	106307	4.23%	0.593%

LSC Area Percent Report

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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
72-12016

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.092	2206	2211	2214	rBV	163998	249811	9.94%	1.393%
38	15.204	2226	2230	2233	rBV	26075	30303	1.21%	0.169%
39	15.404	2259	2264	2270	rVB	104510	134966	5.37%	0.753%
40	15.468	2270	2275	2281	rBV	136077	169529	6.75%	0.945%
41	15.533	2281	2286	2290	rBV	334665	437937	17.43%	2.442%
42	16.121	2375	2386	2398	rBV7	31019	126440	5.03%	0.705%
43	17.080	2542	2549	2558	rVB3	66370	145086	5.77%	0.809%
44	17.545	2621	2628	2639	rBV2	48473	110919	4.41%	0.618%
45	18.250	2742	2748	2756	rVB2	20976	52660	2.10%	0.294%

Sum of corrected areas: 17933963

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Instrument :
BNA_F
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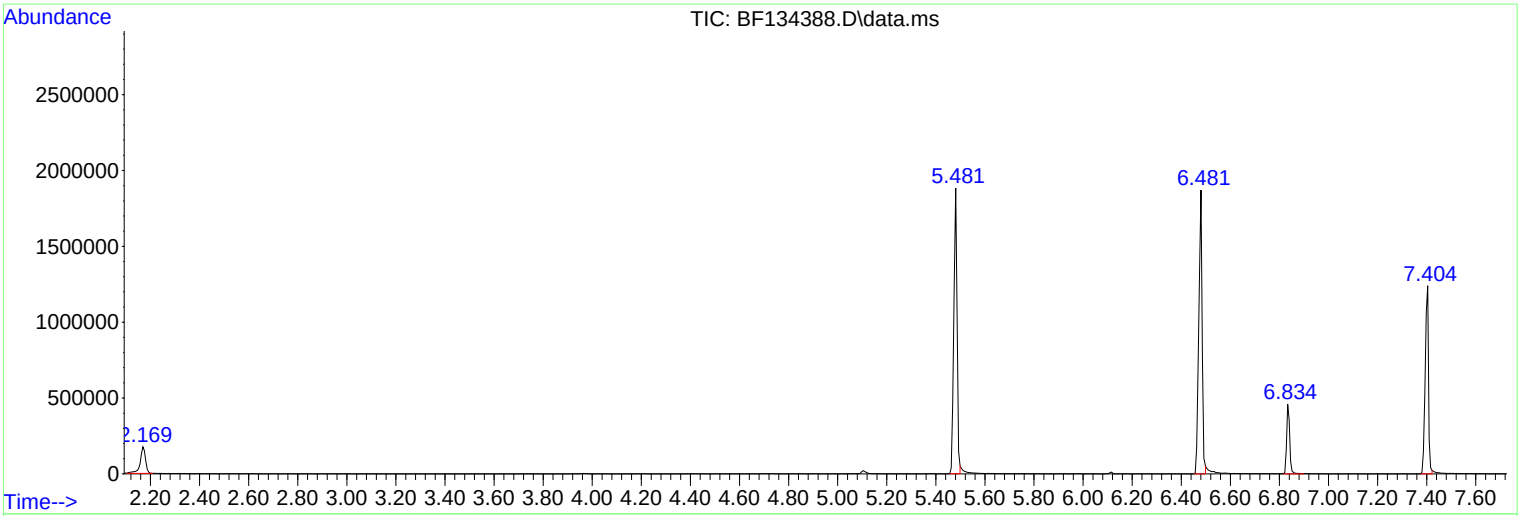
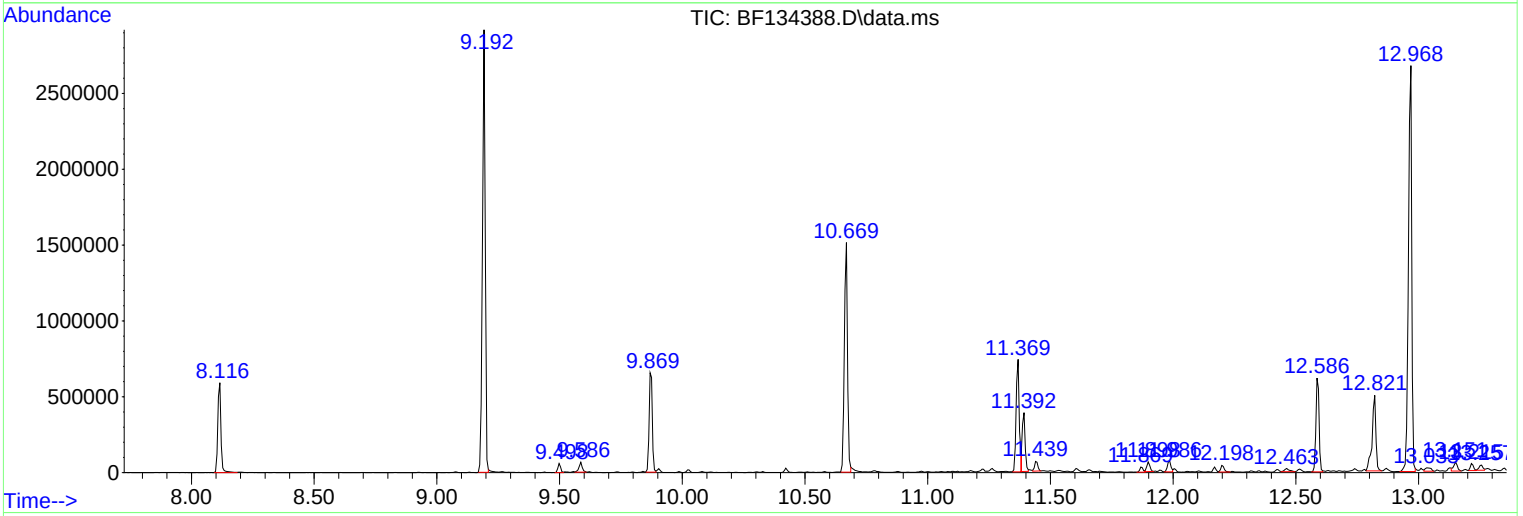
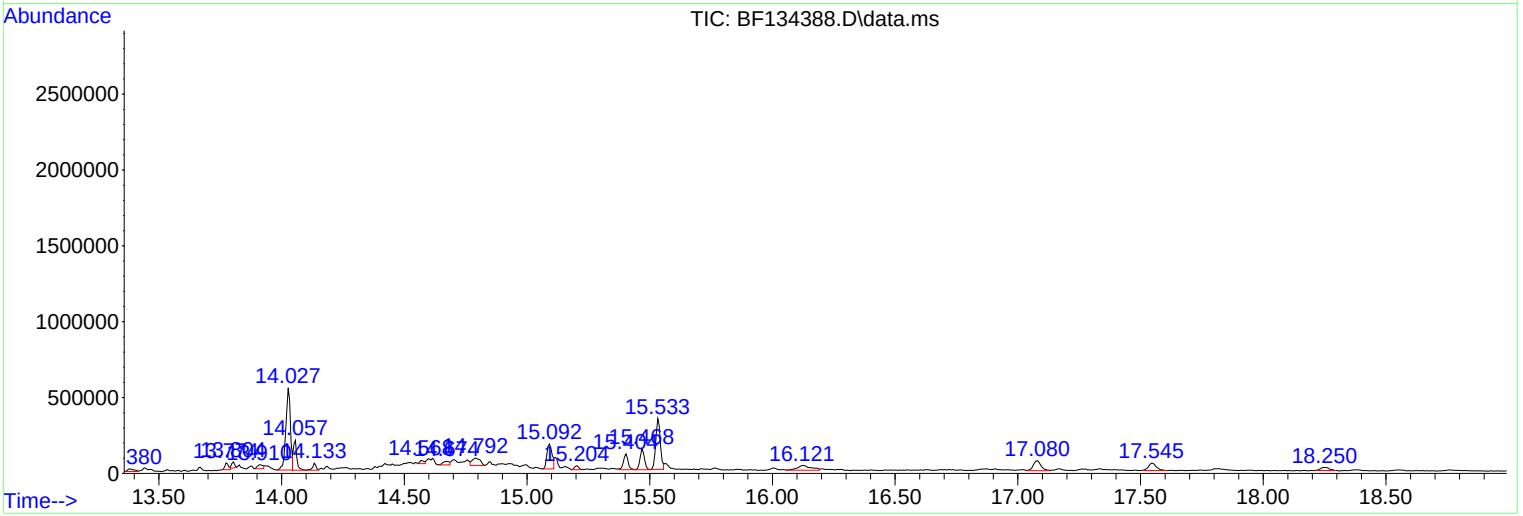
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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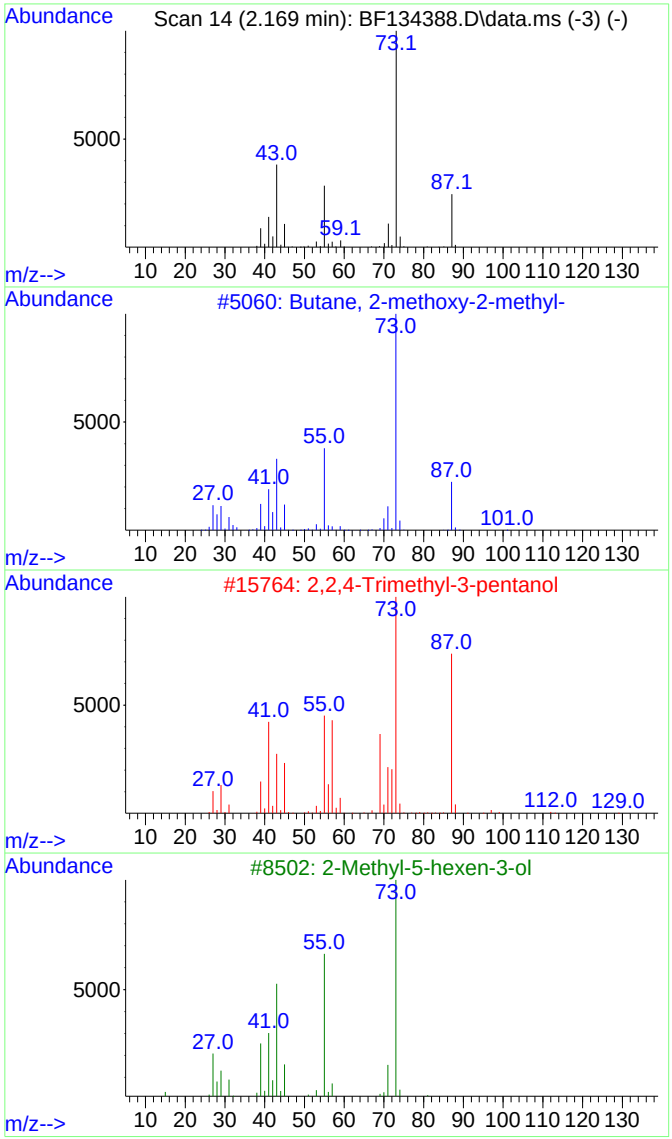
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

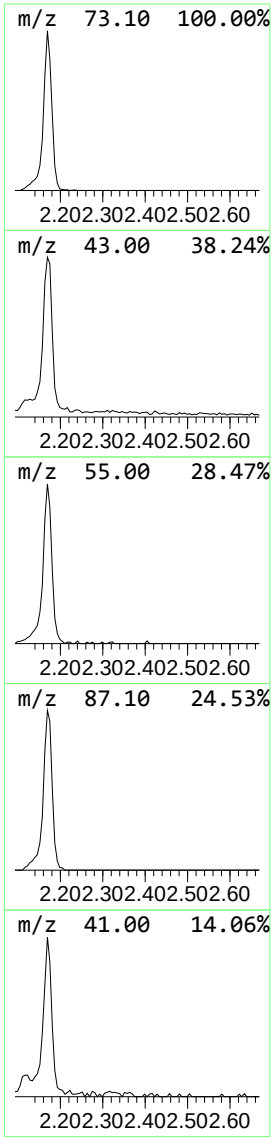
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	13.25 ng	260618	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Instrument :
BNA_F
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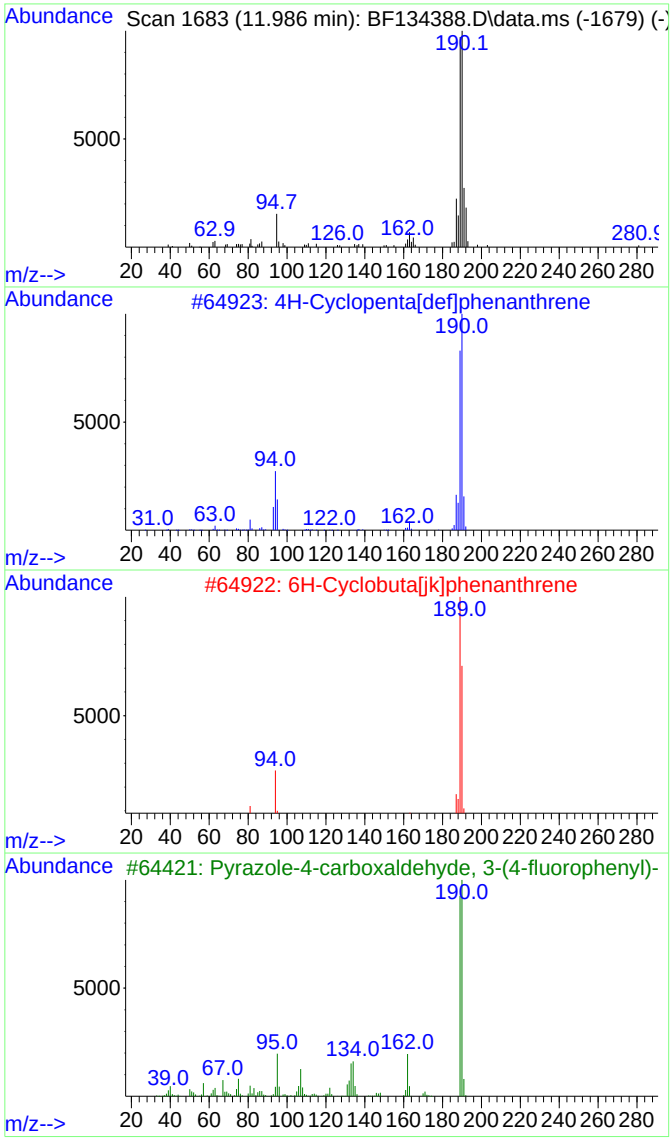
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

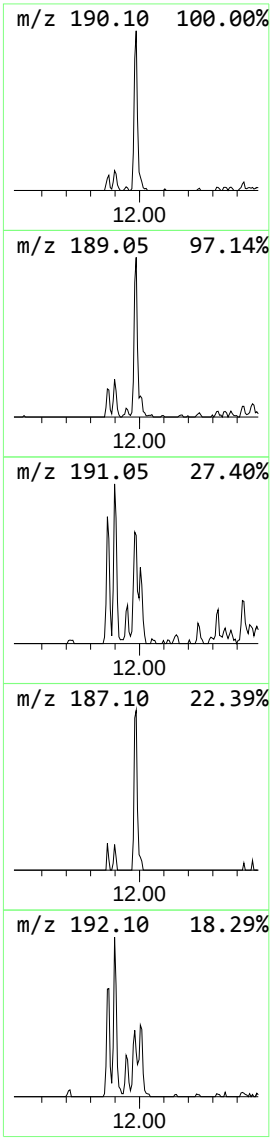
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	2.16 ng	71734	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	53
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	32





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Operator : CG\JU
Sample : 03654-01
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

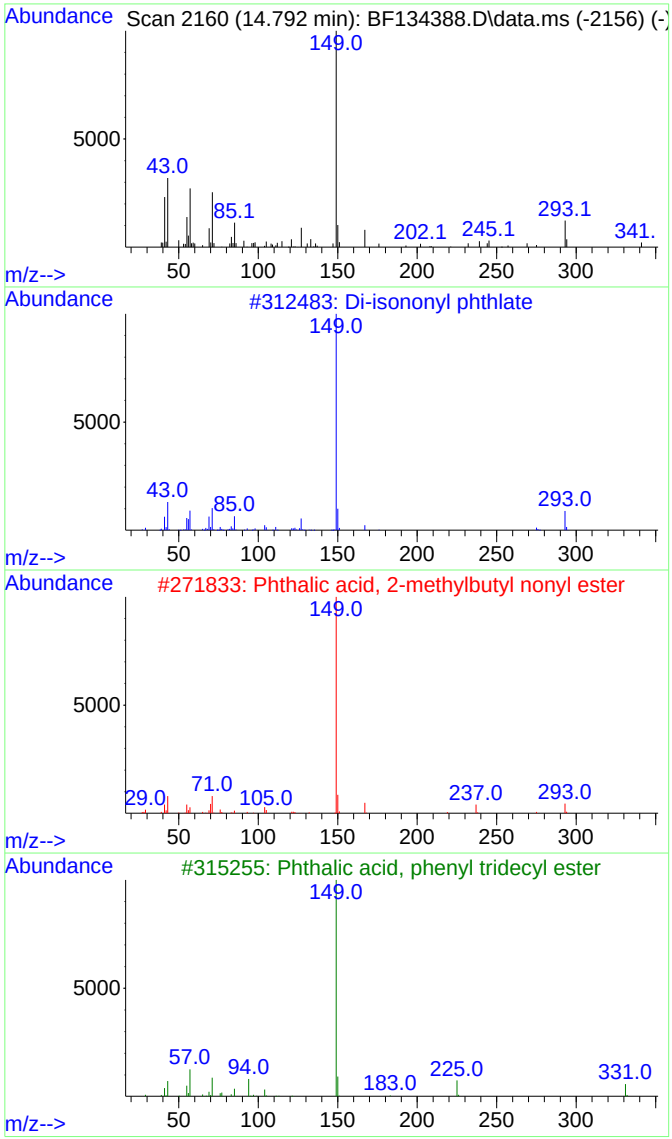
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

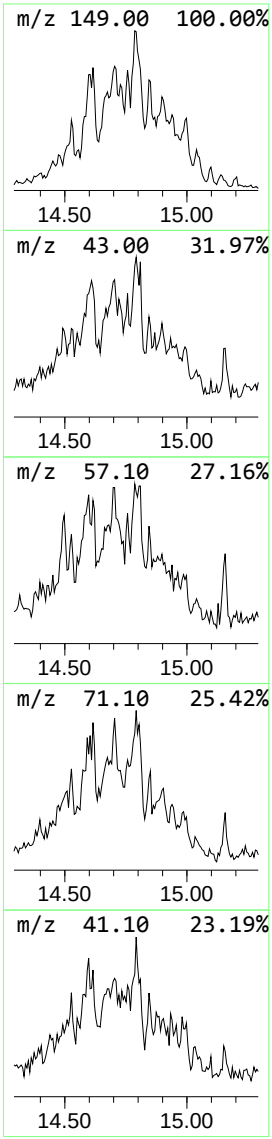
****

Peak Number 3 Di-isononyl phthlate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	4.85 ng	106307	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-isononyl phthlate	418	C26H42O4	020548-62-3	72
2	Phthalic acid, 2-methylbutyl non...	362	C22H34O4	1000322-81-7	64
3	Phthalic acid, phenyl tridecyl e...	424	C27H36O4	1000314-87-8	59
4	Phthalic acid, nonyl tridec-2-yn...	470	C30H46O4	1000315-44-2	59
5	Phthalic acid, 5-methoxy-3-methy...	406	C24H38O5	1000314-89-0	59





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

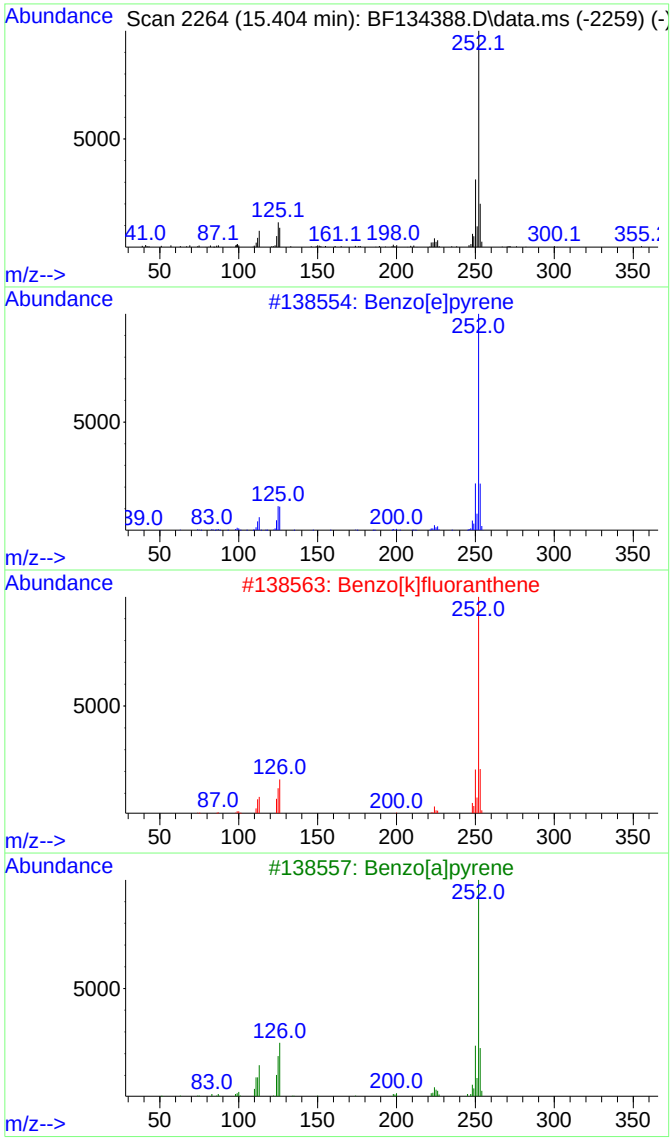
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

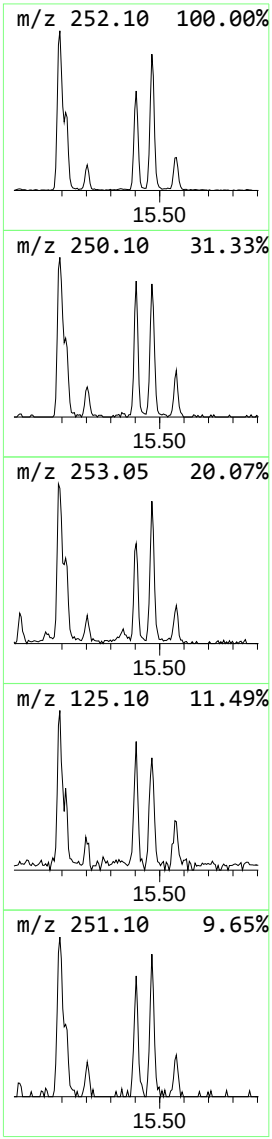
****

Peak Number 4 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	6.16 ng	134966	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5	Perylene	252	C20H12	000198-55-0	90





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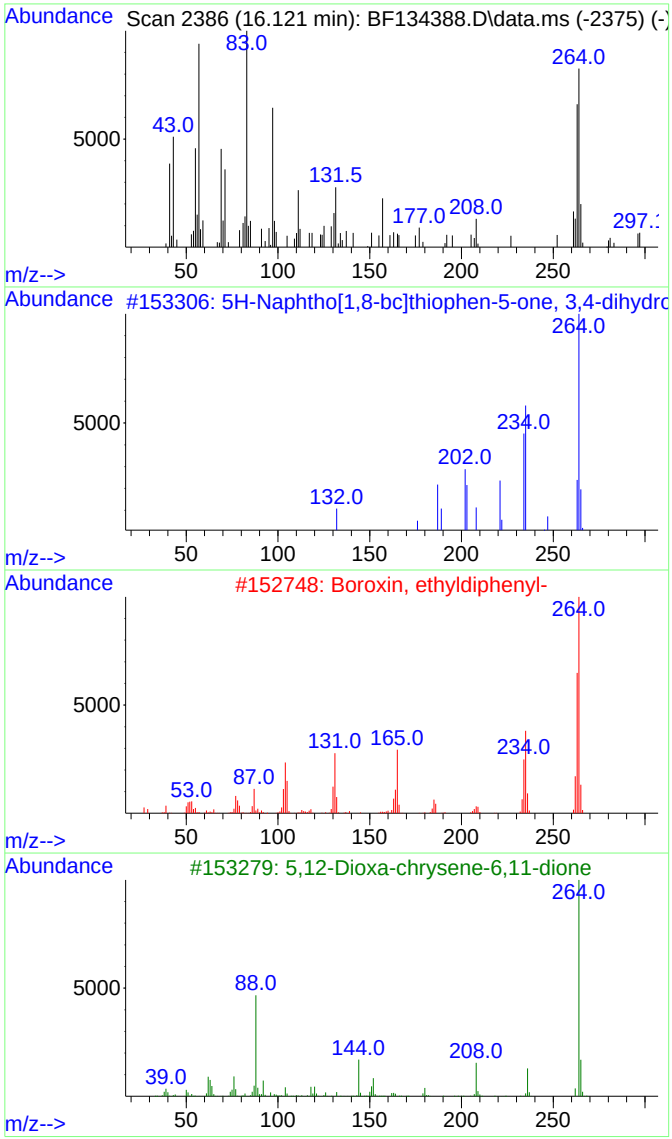
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

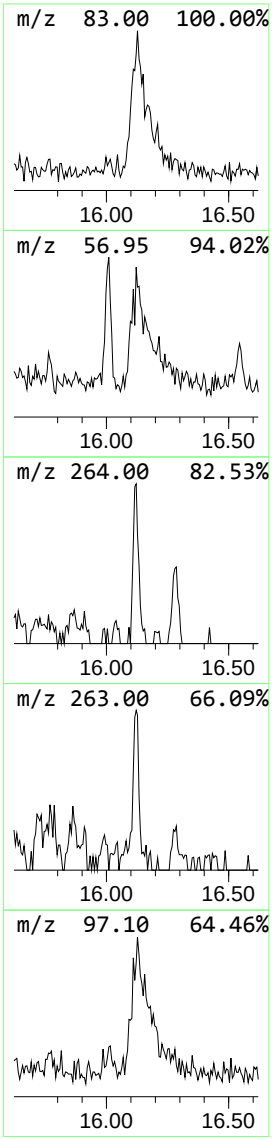
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 5H-Naphtho[1,8-bc]thiophen-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	5.77 ng	126440	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Naphtho[1,8-bc]thiophen-5-one...	264	C17H12OS	010245-65-5	50
2	Boroxin, ethyldiphenyl-	264	C14H15B3O3	1000151-82-0	38
3	5,12-Dioxa-chrysene-6,11-dione	264	C16H8O4	002288-98-4	25
4	2,3,9,10-Tetrahydro-1,8-dioxa-7,...	264	C16H12N2O2	1010243-33-3	22
5	1H,5H-Pyrrolo[1',2':3,4]imidazo[...	166	C10H18N2	054966-11-9	22





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

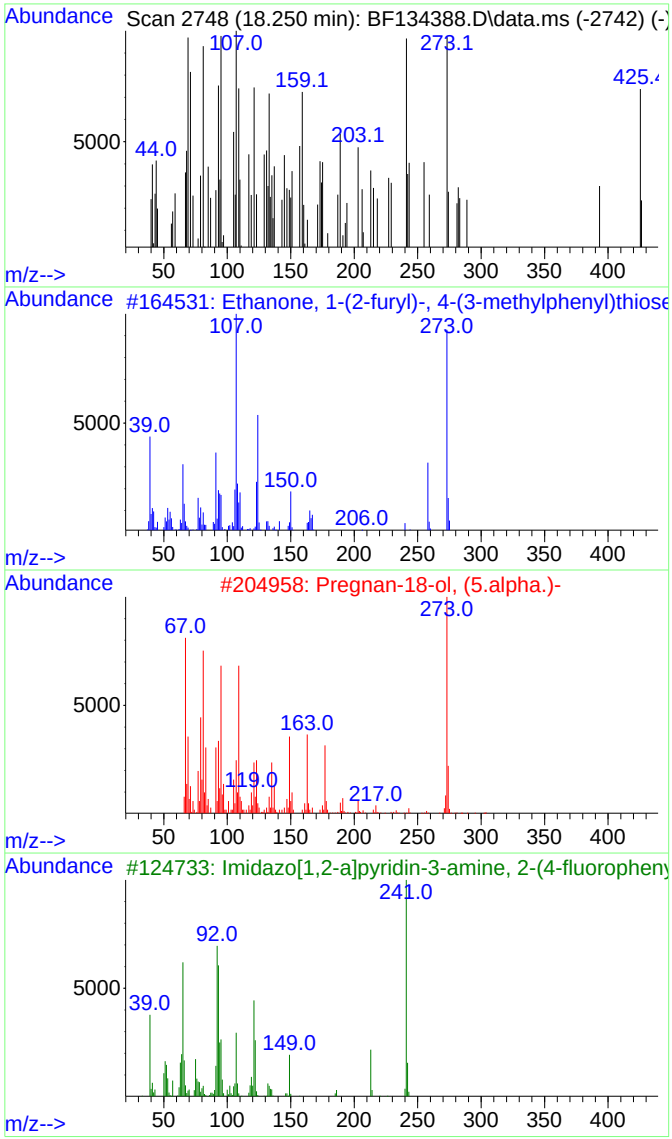
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

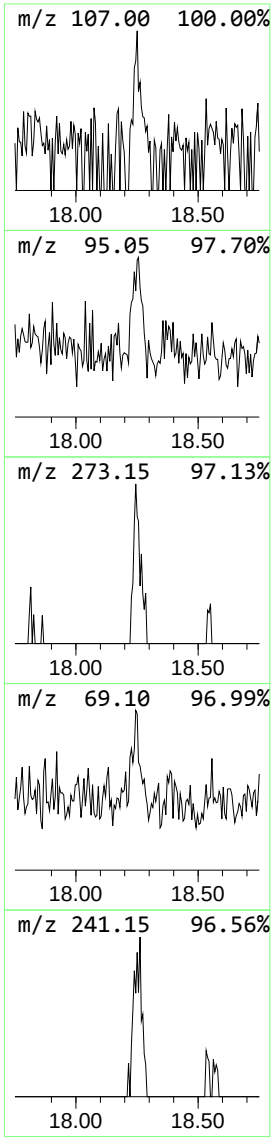
****

Peak Number 6 unknown18.250 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.250	2.40 ng	52660	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2-furyl)-, 4-(3-met...	273	C14H15N3OS	324055-34-7	18
2	Pregnan-18-ol, (5.alpha.)-	304	C21H36O	056053-09-9	16
3	Imidazo[1,2-a]pyridin-3-amine, 2...	241	C14H12FN3	1000318-92-3	14
4	5-[(4-Fluorophenyl)methyl]-2-met...	241	C15H12FNO	1000410-11-7	14
5	2-Pentenoic acid, 5-(decahydro-5...	304	C20H32O2	024470-48-2	12





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
Butane, 2-metho...	2.169	13.3	ng	260618	1	6.834	393484	20.0
4H-Cyclopenta[d...	11.986	2.2	ng	71734	4	11.369	663094	20.0
Di-isononyl pht...	14.792	4.8	ng	106307	6	15.533	437937	20.0
Benzo[e]pyrene	15.404	6.2	ng	134966	6	15.533	437937	20.0
5H-Naphtho[1,8-...	16.121	5.8	ng	126440	6	15.533	437937	20.0
unknown18.250	18.250	2.4	ng	52660	6	15.533	437937	20.0