LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136365.D
Acq On : 02 Dec 2023 07:20
Operator : CG\JU
Sample : 05521-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3-COMP

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: BF136365.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rVB	338451	406079	21.27%	2.527%
2	5.046	498	503	509	rBV	44585	56481	2.96%	0.352%
3	5.446	566	571	574	rBV	2271039	1909273	100.00%	11.882%
4	6.440	735	740	743	rBV	1938770	1697617	88.91%	10.565%
5	6.804	799	802	806	rBV	875946	670085	35.10%	4.170%
6	7.363	892	897	900	rBV	1254218	1049704	54.98%	6.533%
7	8.081	1015	1019	1023	rBV	924680	732430	38.36%	4.558%
8	9.157	1198	1202	1215	rBV	1811360	1553967	81.39%	9.671%
9	9.281	1220	1223	1231	rVB	23737	27881	1.46%	0.174%
10	9.839	1312	1318	1321	rBV	720945	608632	31.88%	3.788%
11	10.628	1448	1452	1464	rBV	952487	835775	43.77%	5.201%
12	11.328	1568	1571	1574	rBV	712004	616788	32.30%	3.839%
13	11.351	1574	1575	1579	rVV	151918	103137	5.40%	0.642%
14	11.404	1581	1584	1588	rVB	38348	31475	1.65%	0.196%
15	11.833	1654	1657	1659	rBV	43013	35528	1.86%	0.221%
16	11.869	1659	1663	1667	rVV2	199079	199848	10.47%	1.244%
17	11.945	1673	1676	1678	rBV2	63324	64283	3.37%	0.400%
18	11.969	1678	1680	1686	rVB	41142	36421	1.91%	0.227%
19	12.133	1702	1708	1710	rBV2	26603	36173	1.89%	0.225%
20	12.280	1727	1733	1736	rBV4	17321	22554	1.18%	0.140%
21	12.386	1747	1751	1754	rBV	45092	42211	2.21%	0.263%
22	12.422	1754	1757	1759	rVV2	28041	29594	1.55%	0.184%
23	12.469	1763	1765	1771	rBV2	33473	38208	2.00%	0.238%
24	12.545	1775	1778	1782	rBV	330692	284330	14.89%	1.770%
25	12.598	1784	1787	1793	rVB5	29833	34052	1.78%	0.212%
26	12.657	1793	1797	1802	rBV5	41392	54991	2.88%	0.342%
27	12.774	1814	1817	1820	rVB	353001	322339	16.88%	2.006%
28	12.827	1824	1826	1830	rVB2	28065	31566	1.65%	0.196%
29	12.927	1839	1843	1846	rBV	2126578	1725635	90.38%	10.740%
30	12.998	1850	1855	1863	rVB3	33730	50051	2.62%	0.311%
31	13.086	1867	1870	1871	rBV3	24923	29474	1.54%	0.183%
32	13.110	1871	1874	1877	rVB	50895	53752	2.82%	0.335%
33	13.174	1877	1885	1888	rBV2	41684	56238	2.95%	0.350%
34	13.210	1888	1891	1894	rBV	52613	52049	2.73%	0.324%
35	13.304	1904	1907	1910	rBV	33366	34498	1.81%	0.215%
36	13.333	1910	1912	1916	rVB	31849	30537	1.60%	0.190%

LSC Area Percent Report

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Acq On : 02 Dec 2023 07:20
Operator : CG\JU
Sample : 05521-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-COMP

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	13.463	1931	1934	1936	rBV	43863	34958	1.83%	0.218%
38	13.616	1953	1960	1966	rBV2	33401	75152	3.94%	0.468%
39	13.727	1973	1979	1982	rBV5	25292	40636	2.13%	0.253%
40	13.839	1993	1998	2003	rVB3	26052	41340	2.17%	0.257%
41	13.910	2005	2010	2012	rBV4	34995	57710	3.02%	0.359%
42	13.980	2017	2022	2025	rVV2	792759	906414	47.47%	5.641%
43	14.010	2025	2027	2032	rVB	158203	143126	7.50%	0.891%
44	14.163	2049	2053	2057	rVB5	30401	35884	1.88%	0.223%
45	14.374	2085	2089	2092	rVB	38750	40431	2.12%	0.252%
46	14.463	2098	2104	2107	rBV4	58240	77413	4.05%	0.482%
47	14.780	2156	2158	2166	rVB3	23849	30982	1.62%	0.193%
48	14.857	2167	2171	2175	rVV	51710	60819	3.19%	0.379%
49	15.027	2196	2200	2203	rBV	92042	134283	7.03%	0.836%
50	15.133	2214	2218	2223	rVB2	32558	53316	2.79%	0.332%
51	15.339	2249	2253	2259	rVB	46612	58666	3.07%	0.365%
52	15.398	2259	2263	2269	rVB	71291	86732	4.54%	0.540%
53	15.468	2269	2275	2279	rBV	417246	534705	28.01%	3.328%
54	15.980	2357	2362	2367	rVB3	21342	38134	2.00%	0.237%
55	16.968	2526	2530	2539	rVB3	23613	53751	2.82%	0.335%

Sum of corrected areas: 16068108

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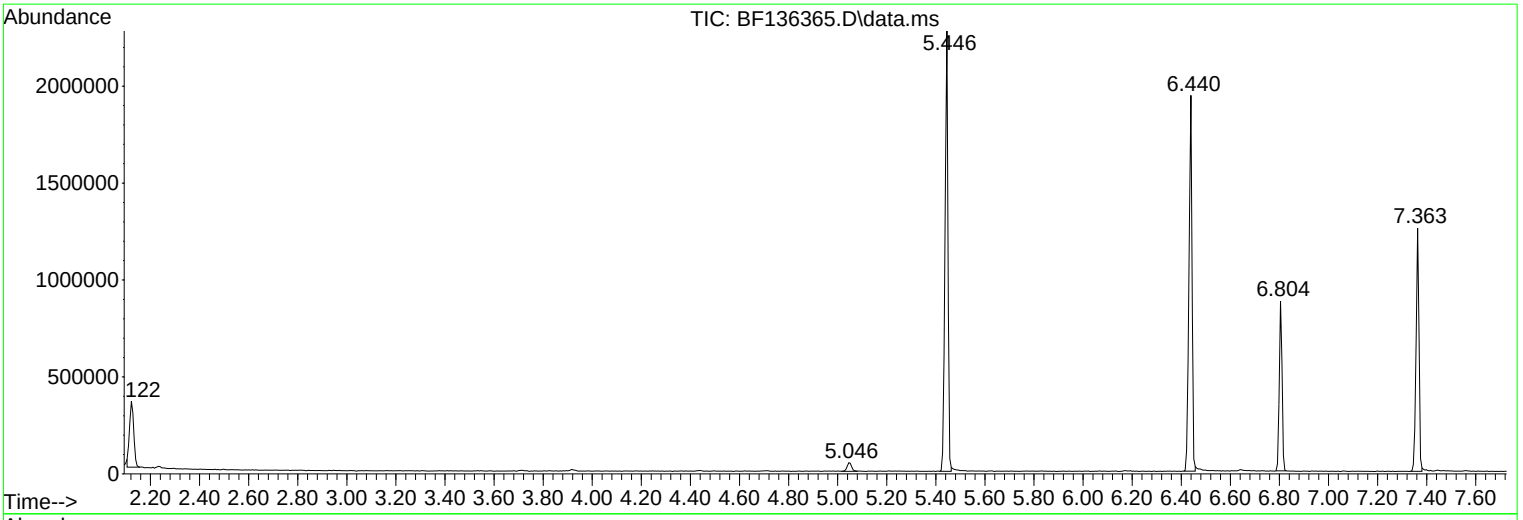
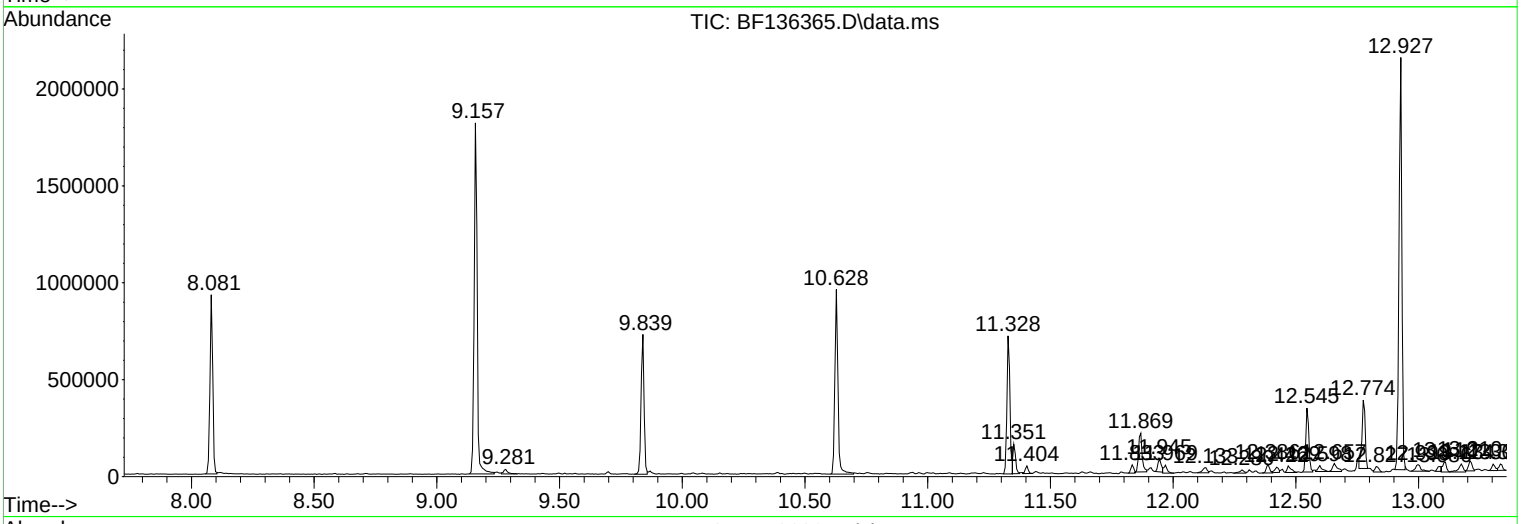
ALS Vial : 36 Sample Multiplier: 1

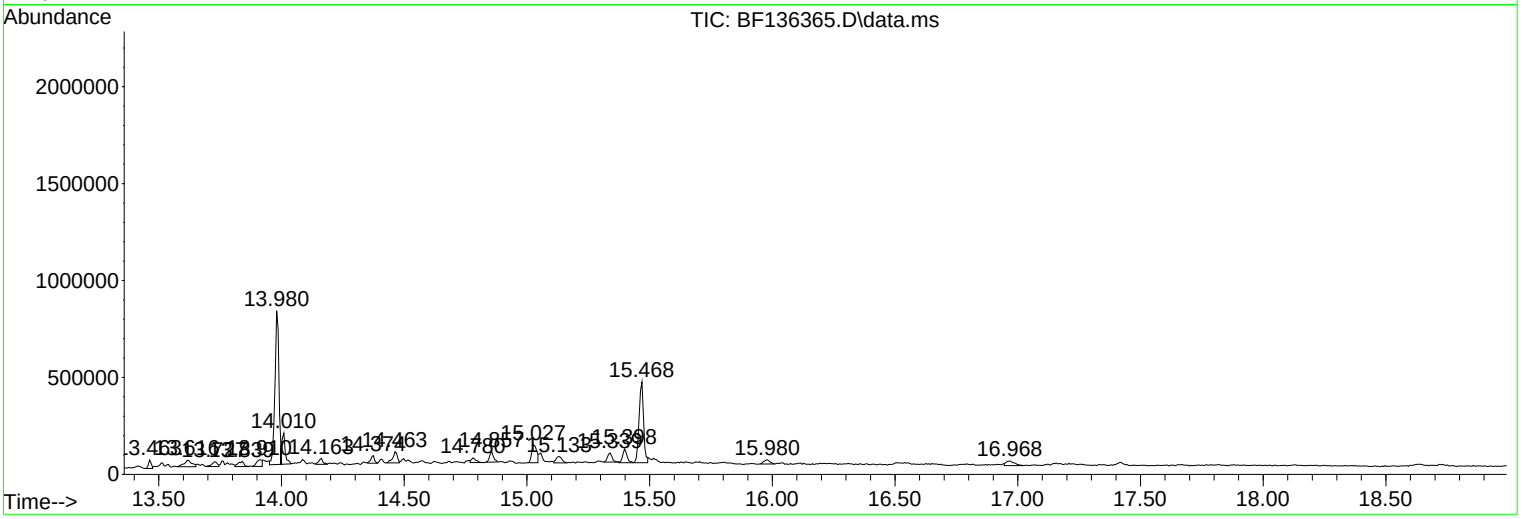
Instrument :
BNA_F
ClientSampleId :
SP-3-COMP

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
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Operator : CG\JU
Sample : 05521-07
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Instrument :
BNA_F
ClientSampleId :
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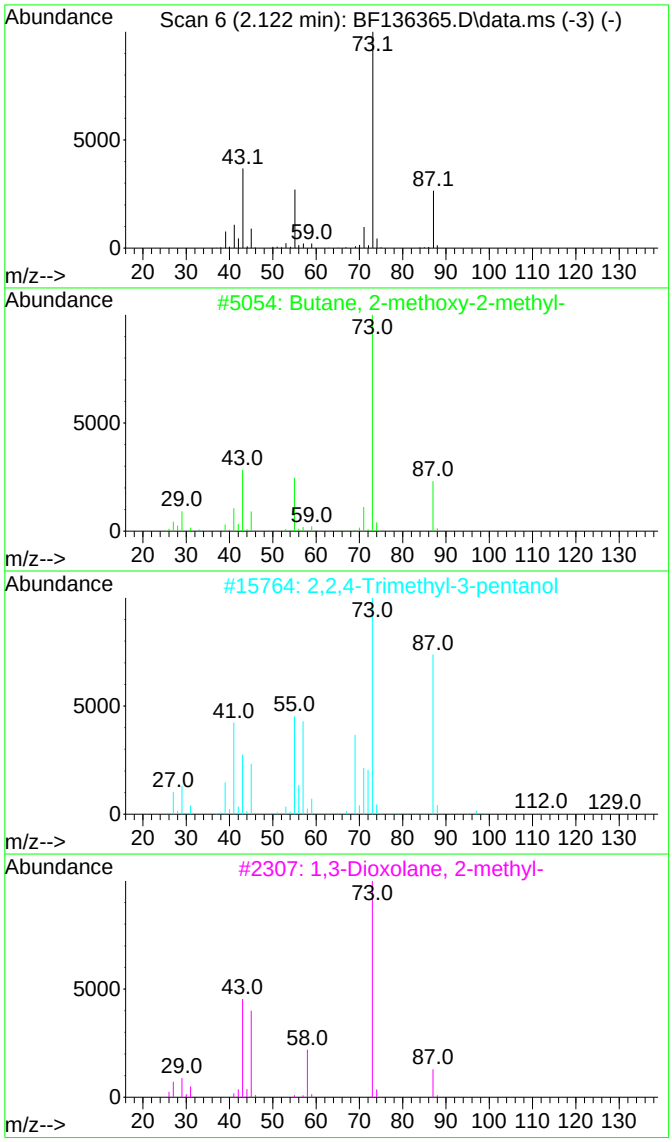
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

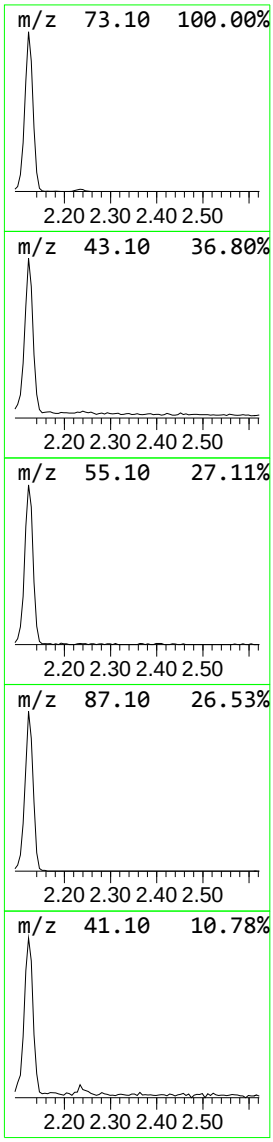
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	12.12 ng	406079	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Data File : BF136365.D
Acq On : 02 Dec 2023 07:20
Operator : CG\JU
Sample : 05521-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-COMP

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

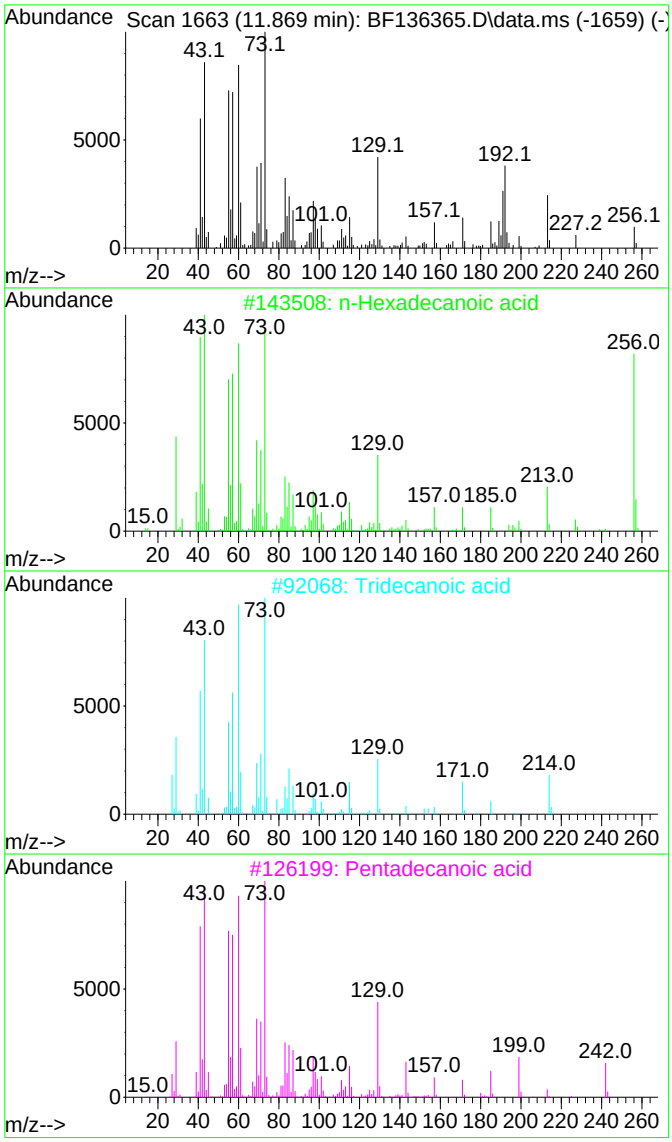
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

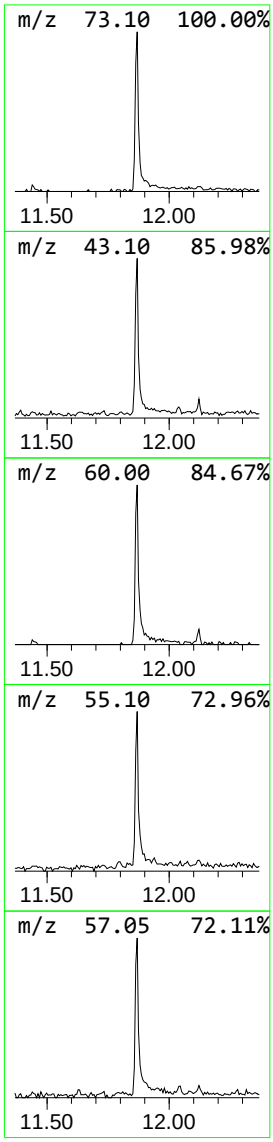
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	6.48 ng	199848	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
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Acq On : 02 Dec 2023 07:20
Operator : CG\JU
Sample : 05521-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-COMP

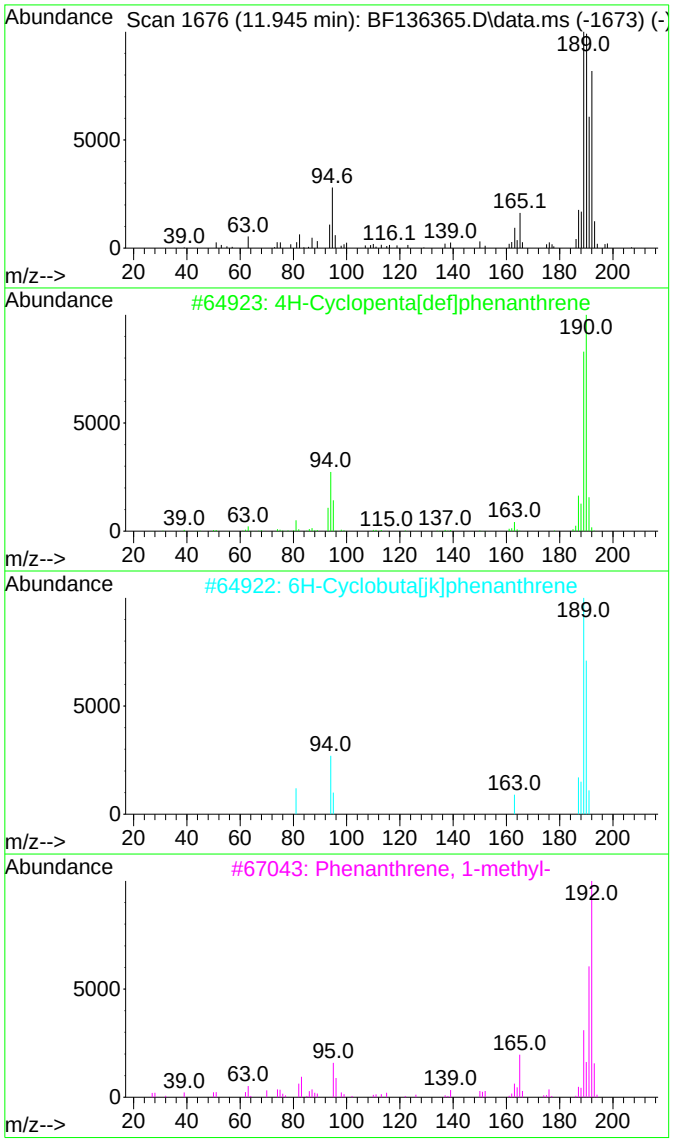
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

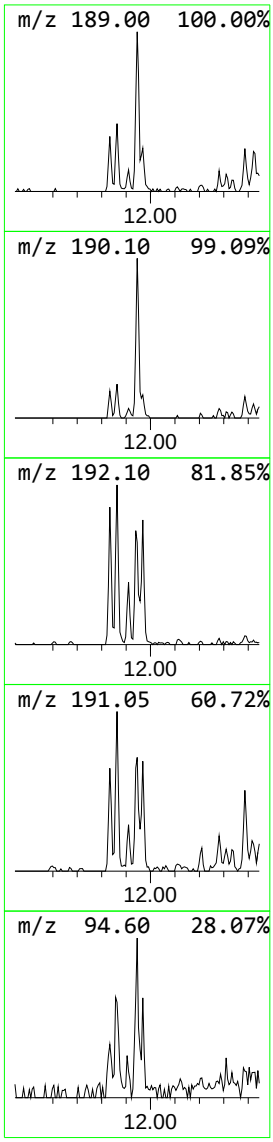
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.08 ng	64283	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
4	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	41
5	3-Bromo-2-furoic acid	190	C5H3BrO3	014903-90-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
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Sample : 05521-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3-COMP

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

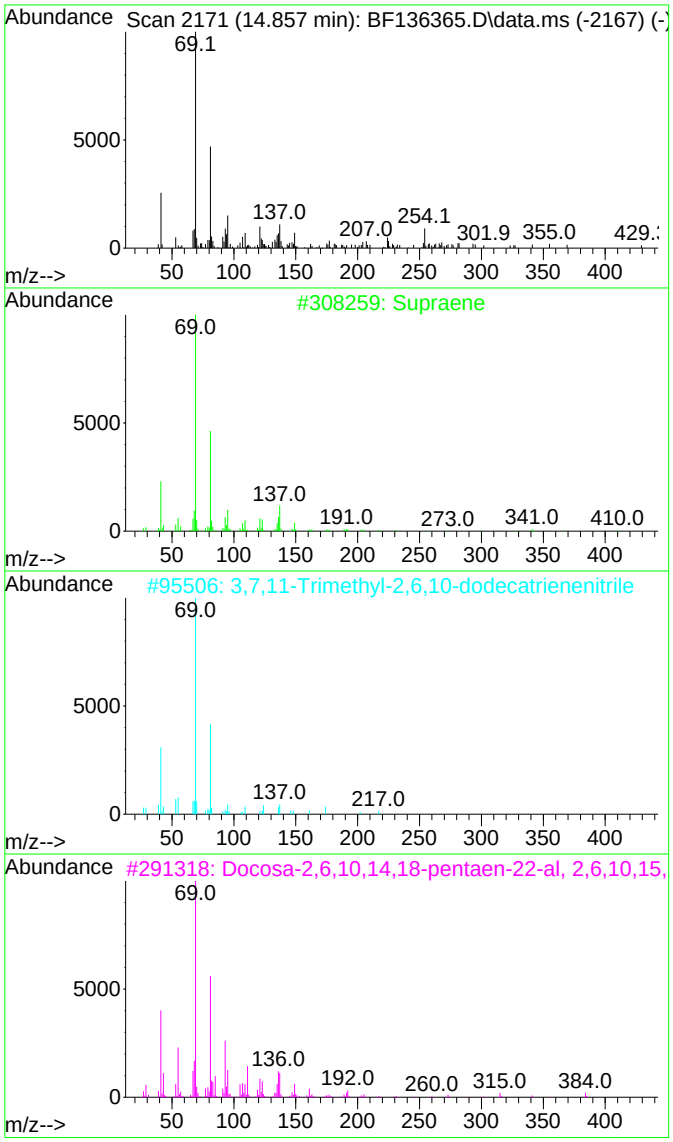
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

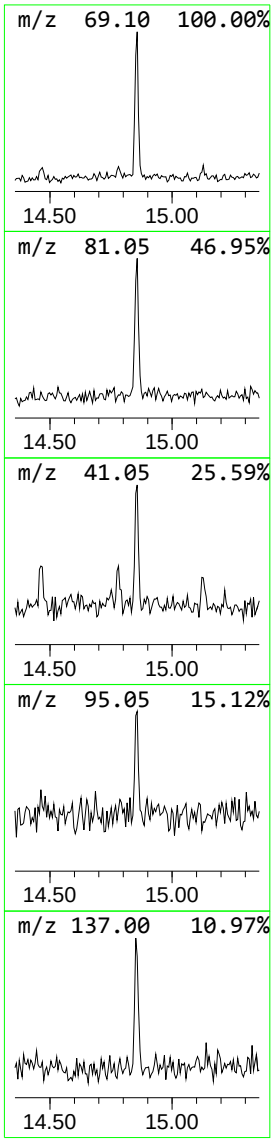
****

Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	2.27 ng	60819	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	72
2	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	53
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	50
4	2-propenamide, 2-methyl-N-[4-[(m...	254	C11H14N2O3S	1000401-43-5	50
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50





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

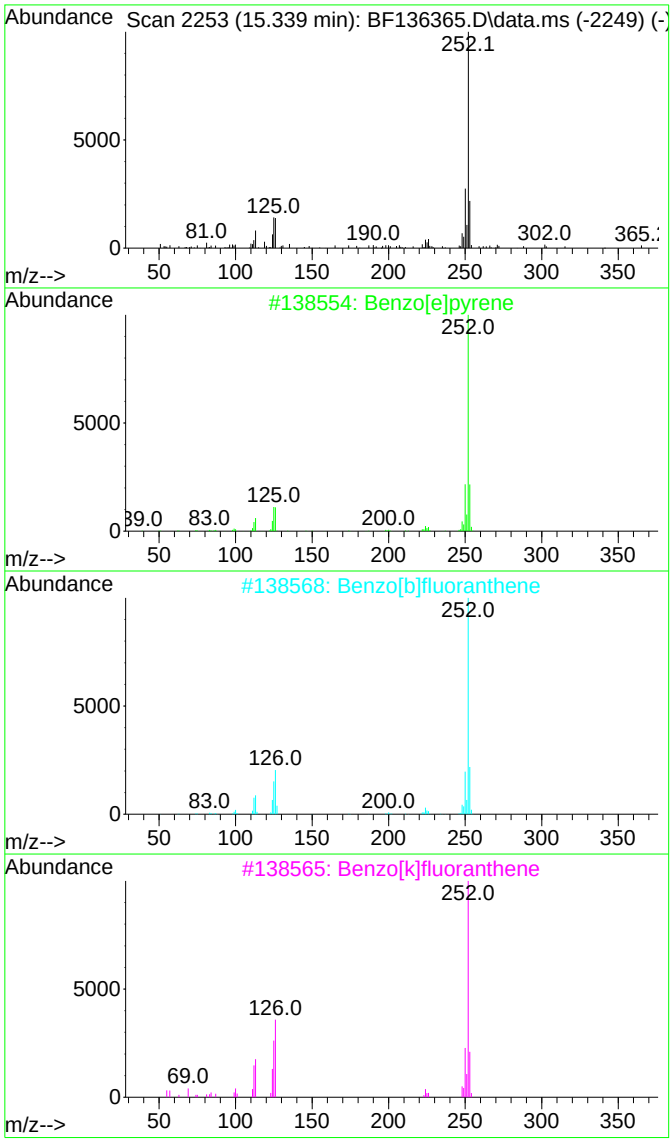
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

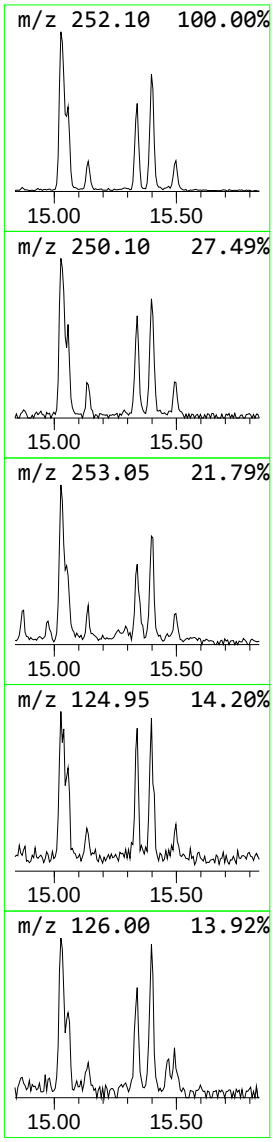
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	2.19 ng	58666	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

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Instrument :
BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.122	12.1	ng	406079	1	6.804	670085	20.0
n-Hexadecanoic ...	11.869	6.5	ng	199848	4	11.328	616788	20.0
4H-Cyclopenta[d...	11.945	2.1	ng	64283	4	11.328	616788	20.0
Supraene	14.857	2.3	ng	60819	6	15.468	534705	20.0
Benzo[e]pyrene	15.339	2.2	ng	58666	6	15.468	534705	20.0