LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103276.D
Acq On : 27 Feb 2018 21:07
Operator : SJ/JU
Sample : J1698-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3

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:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	17	rVB	238325	312911	8.59%	0.978%
2	5.110	511	514	522	rBV	85839	110519	3.03%	0.345%
3	5.498	576	580	604	rBV	3176317	3641849	100.00%	11.381%
4	6.516	747	753	771	rBV	2974817	3610831	99.15%	11.284%
5	6.651	771	776	779	rBV	3254199	3443475	94.55%	10.761%
6	6.875	810	814	821	rBV	1233318	992354	27.25%	3.101%
7	7.033	836	841	844	rBV	2830497	2641969	72.54%	8.256%
8	7.186	864	867	875	rVB	50466	48747	1.34%	0.152%
9	7.404	900	904	906	rBV	45966	38001	1.04%	0.119%
10	7.439	906	910	913	rBV	2287410	2207665	60.62%	6.899%
11	7.663	946	948	952	rVB	51609	47352	1.30%	0.148%
12	7.892	983	987	989	rBV	45345	39260	1.08%	0.123%
13	8.157	1028	1032	1039	rBV	1417203	1284625	35.27%	4.015%
14	9.233	1210	1215	1218	rBV	3472524	3237600	88.90%	10.118%
15	9.298	1224	1226	1230	rVB	64441	58983	1.62%	0.184%
16	9.574	1265	1273	1276	rBV4	23635	38214	1.05%	0.119%
17	9.622	1277	1281	1289	rVB	420191	394619	10.84%	1.233%
18	9.774	1303	1307	1312	rBV	45345	55062	1.51%	0.172%
19	9.833	1312	1317	1321	rVB	95809	93295	2.56%	0.292%
20	9.916	1327	1331	1335	rBV	1316468	1143924	31.41%	3.575%
21	10.151	1368	1371	1375	rBV3	39451	44043	1.21%	0.138%
22	10.327	1398	1401	1405	rVB	104442	96859	2.66%	0.303%
23	10.463	1421	1424	1431	rVB3	23898	38622	1.06%	0.121%
24	10.551	1433	1439	1441	rBV	57517	65530	1.80%	0.205%
25	10.710	1461	1466	1476	rBV	1415398	1504648	41.32%	4.702%
26	10.804	1479	1482	1491	rVB	108509	165227	4.54%	0.516%
27	11.016	1512	1518	1519	rBV5	23814	40446	1.11%	0.126%
28	11.251	1555	1558	1561	rBV	62790	52926	1.45%	0.165%
29	11.404	1581	1584	1587	rBV	974883	911294	25.02%	2.848%
30	11.427	1587	1588	1595	rVB	148483	119679	3.29%	0.374%
31	11.910	1667	1670	1673	rBV	67573	82015	2.25%	0.256%
32	11.939	1673	1675	1678	rVB	75421	63241	1.74%	0.198%
33	12.021	1686	1689	1691	rBV2	103473	113936	3.13%	0.356%
34	12.045	1691	1693	1698	rVB	71156	60143	1.65%	0.188%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : B3

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:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.457	1760	1763	1765	rBV	90528	89522	2.46%	0.280%
36	12.551	1775	1779	1783	rBV4	40849	72176	1.98%	0.226%
37	12.621	1787	1791	1795	rBV	259678	246690	6.77%	0.771%
38	12.851	1824	1830	1836	rBV	352461	407430	11.19%	1.273%
39	12.904	1836	1839	1843	rVB3	48445	56029	1.54%	0.175%
40	12.992	1850	1854	1857	rBV	2293077	2105697	57.82%	6.580%
41	13.068	1864	1867	1874	rVB5	41850	74933	2.06%	0.234%
42	13.157	1879	1882	1883	rBV3	47387	45395	1.25%	0.142%
43	13.180	1884	1886	1888	rVB2	77874	64240	1.76%	0.201%
44	13.245	1895	1897	1900	rBV	54343	51781	1.42%	0.162%
45	13.286	1901	1904	1907	rBV	67420	66989	1.84%	0.209%
46	13.380	1917	1920	1923	rBV	69199	62877	1.73%	0.196%
47	13.410	1923	1925	1928	rBV	60103	57064	1.57%	0.178%
48	13.874	2000	2004	2008	rBV2	231917	267775	7.35%	0.837%
49	14.057	2030	2035	2038	rBV2	825626	906770	24.90%	2.834%
50	14.080	2038	2039	2047	rVB	154371	126345	3.47%	0.395%
51	14.139	2047	2049	2051	rBV2	50058	43516	1.19%	0.136%
52	15.556	2286	2290	2295	rVB	367060	454166	12.47%	1.419%

Sum of corrected areas: 31999259

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Instrument : BNA_F
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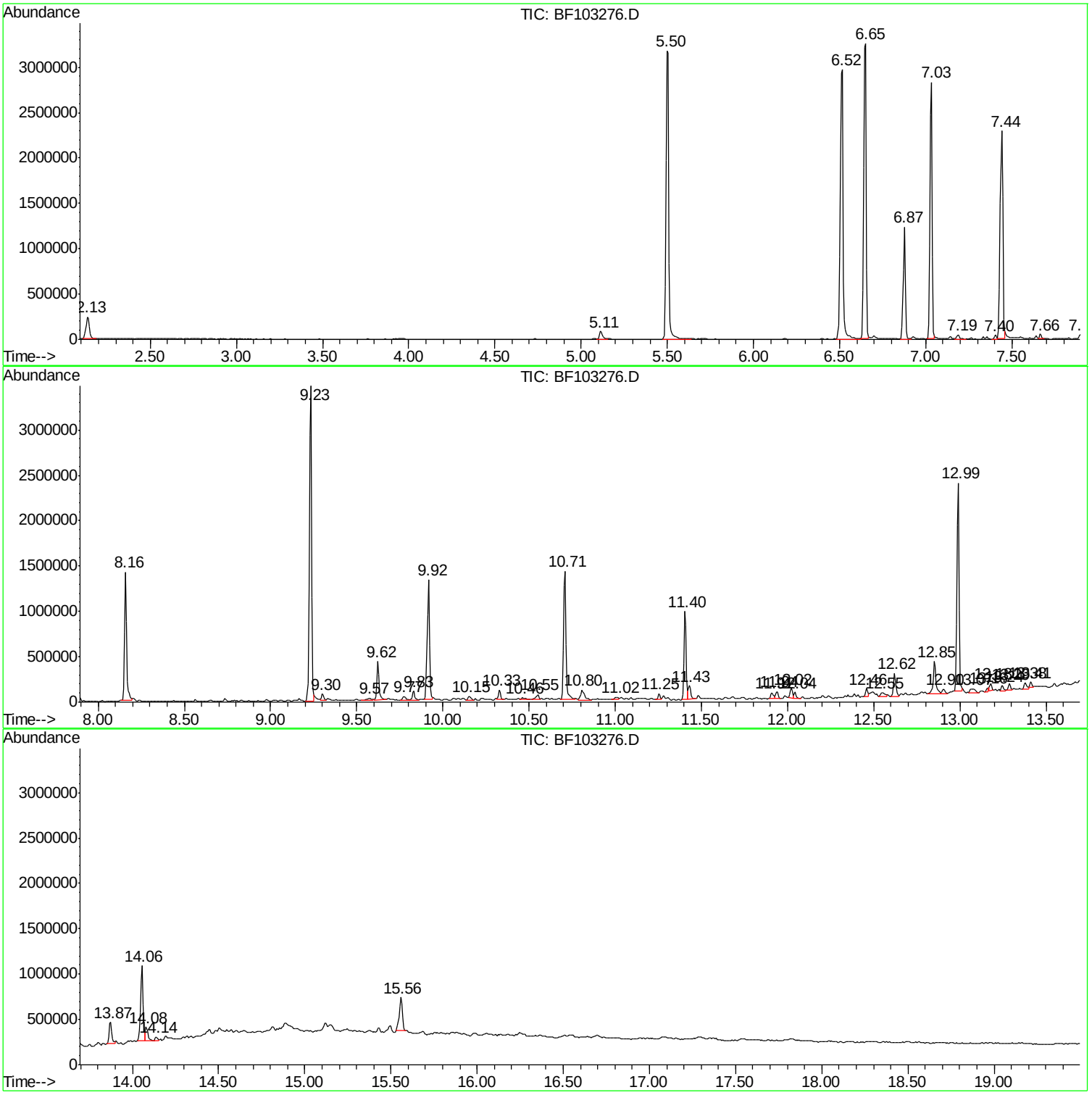
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103276.D
Acq On : 27 Feb 2018 21:07
Operator : SJ/JU
Sample : J1698-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

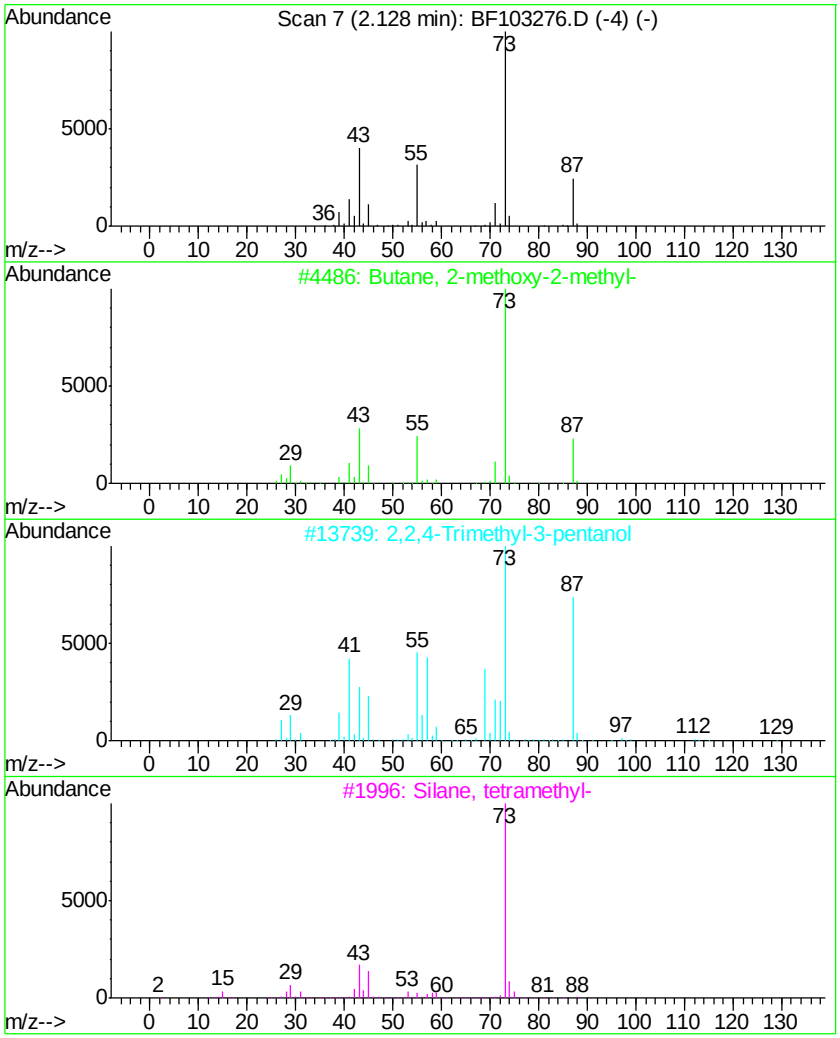
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

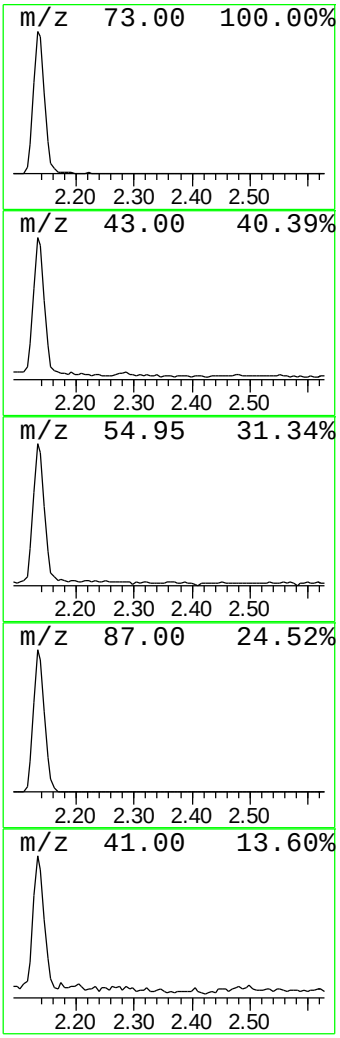
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	6.31 ng	312911	1,4-Dichlorobenzene-d4	6.87

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
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Acq On : 27 Feb 2018 21:07
Operator : SJ/JU
Sample : J1698-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

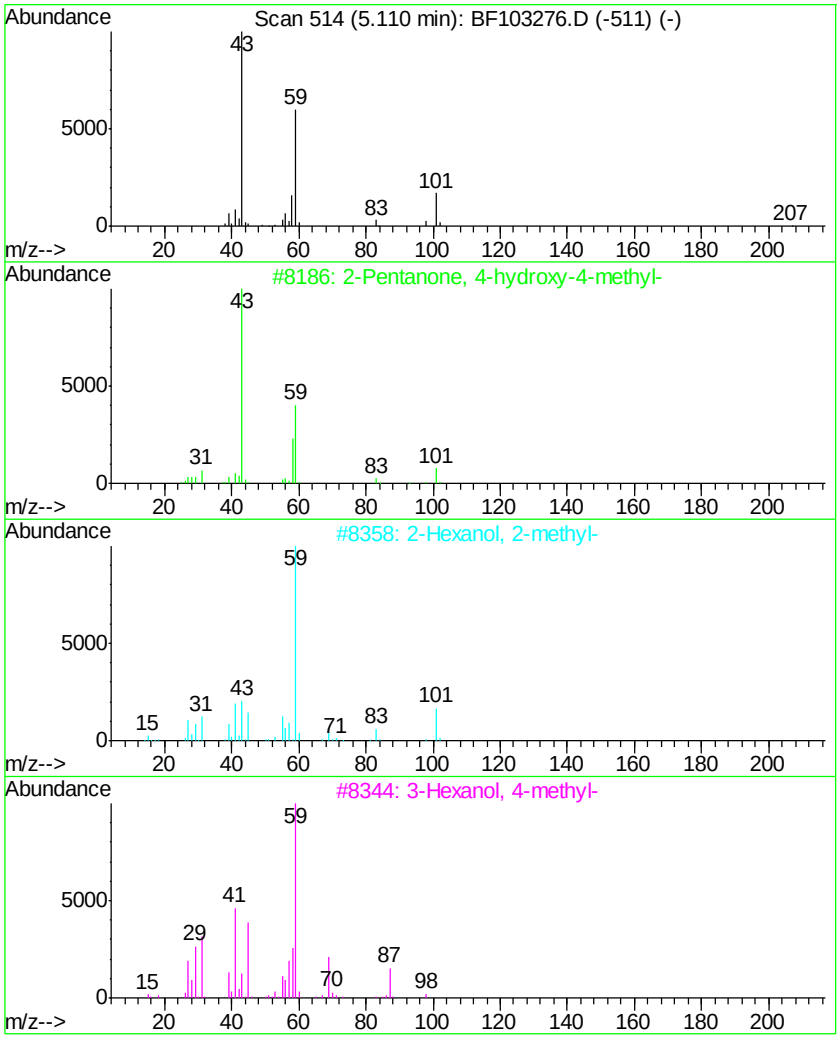
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

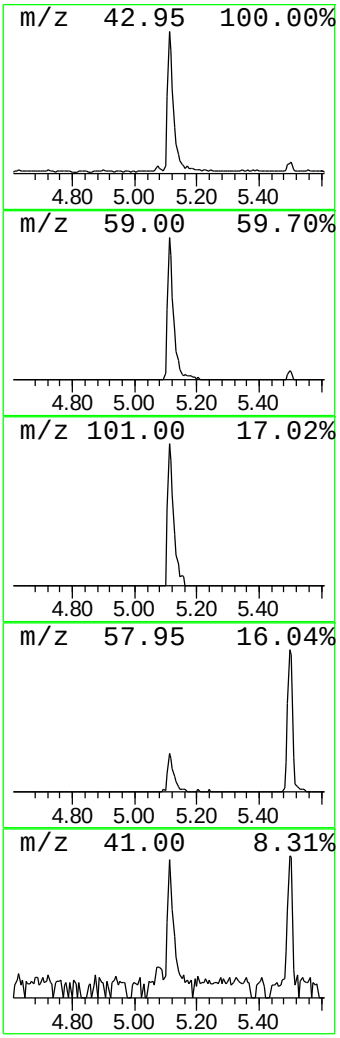
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.23 ng	110519	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23





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Data File : BF103276.D
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Sample : J1698-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

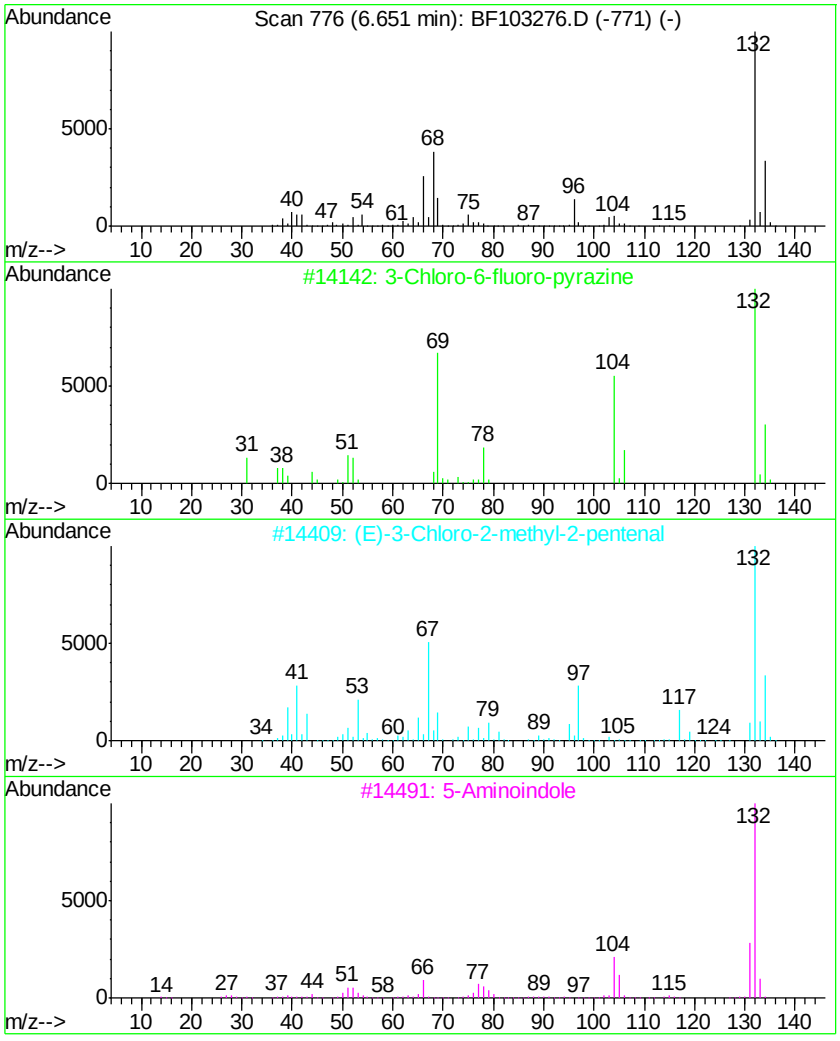
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

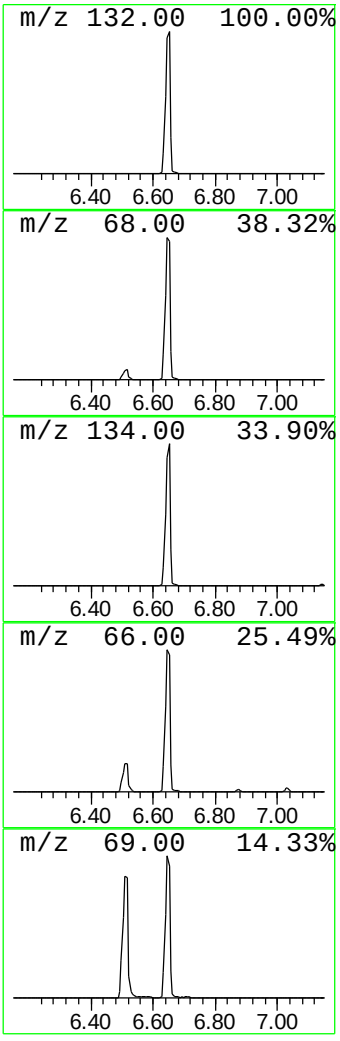
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	69.40 ng	3443480	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Xenon	132	Xe	007440-63-3	9





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Instrument : BNA_F
ClientSampleId : B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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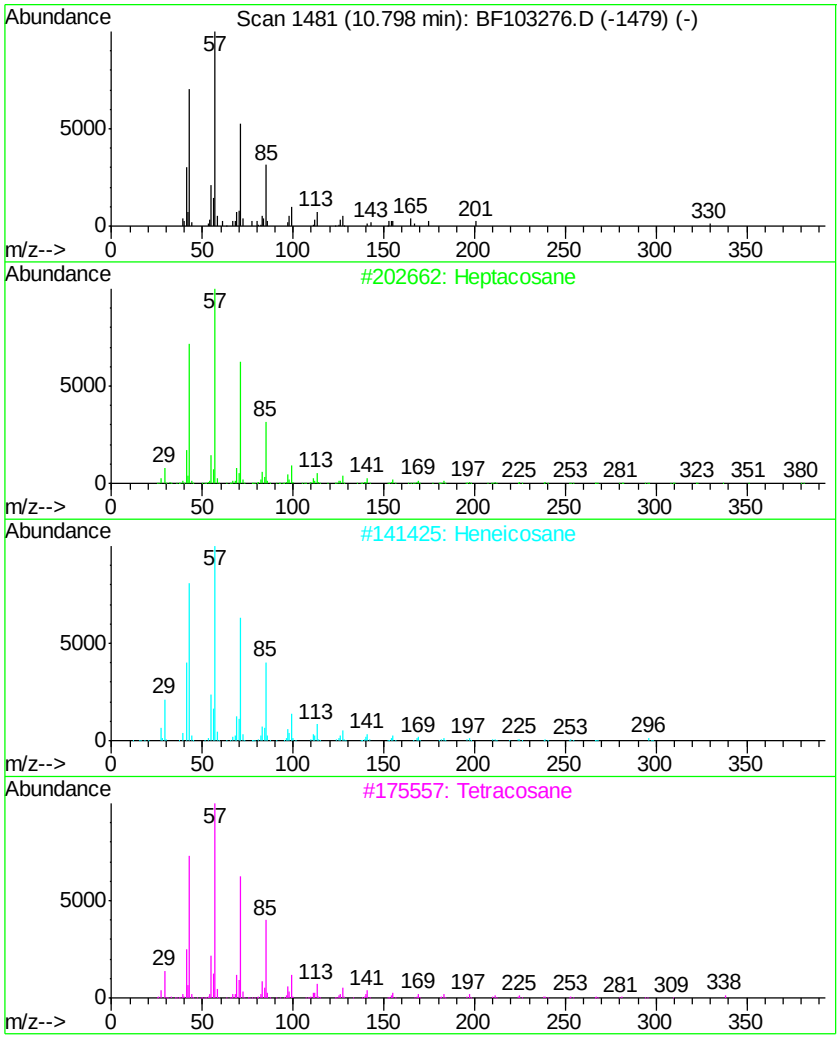
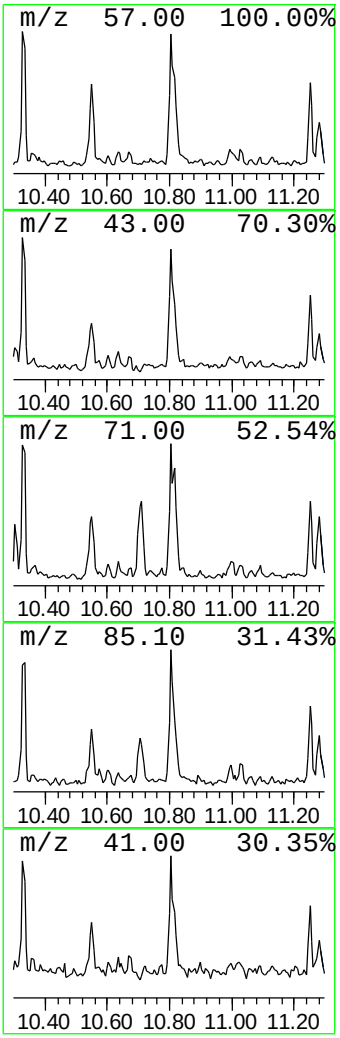
Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	3.63 ng	165227	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptadecane	240	C17H36	000629-78-7	90
5	Tetradecane	198	C14H30	000629-59-4	86





Library Search Compound Report

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Instrument : BNA_F
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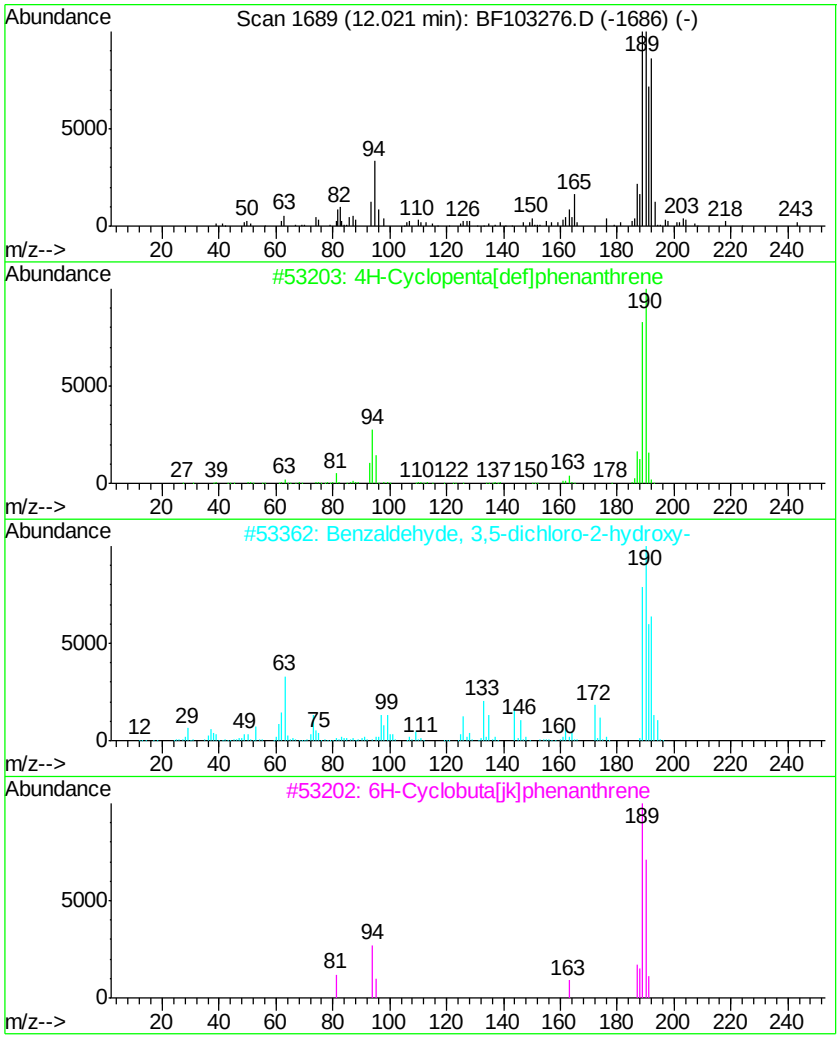
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

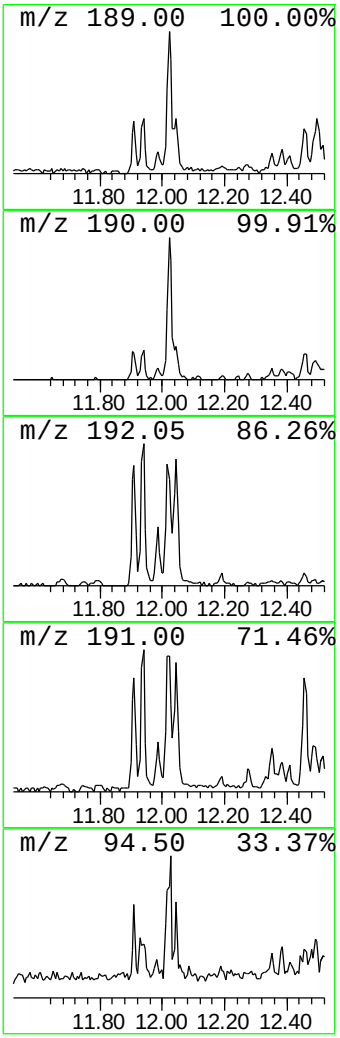
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.50 ng	113936	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	30
5	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	30





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Misc :
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Instrument : BNA_F
ClientSampleId : B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

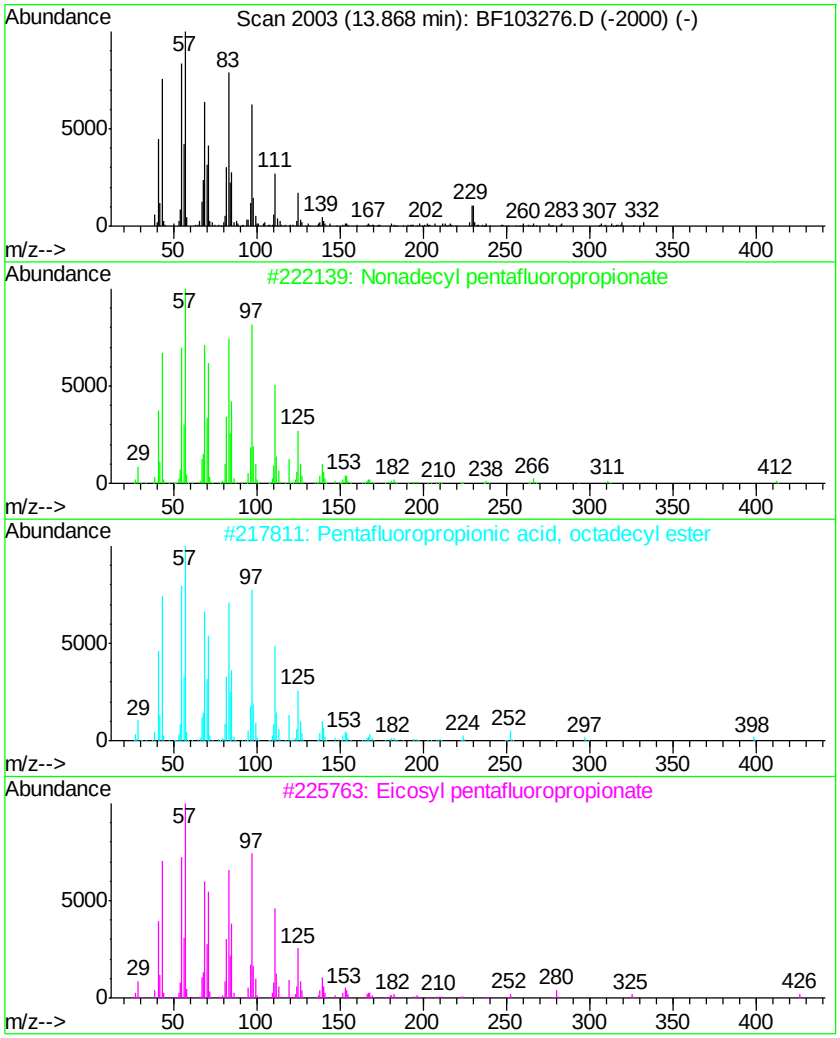
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

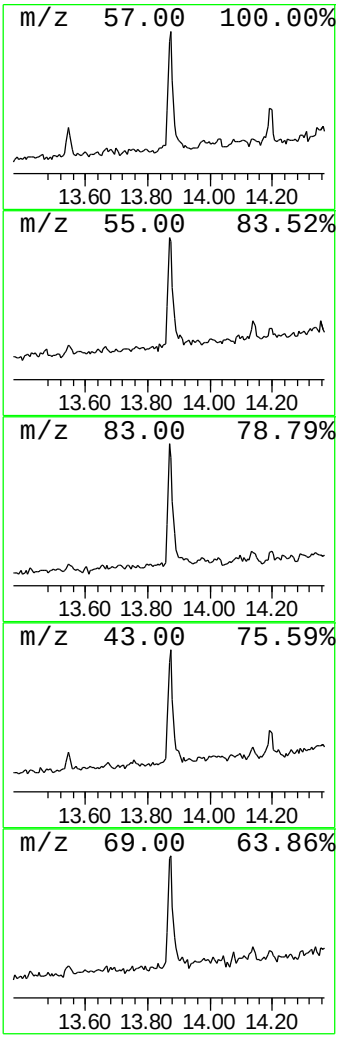
****

Peak Number 7 Nonadecyl pentafluoropropio... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	5.91 ng	267775	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
3	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
5	Carbonic acid, hexadecyl isobuty...	342	C21H42O3	1000314-61-3	91





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	6.3	ng	312911	1	6.87	992354	20.0
2-Pentanone, 4-hy...	5.11	2.2	ng	110519	1	6.87	992354	20.0
unknown6.65	6.65	69.4	ng	3443480	1	6.87	992354	20.0
Heptacosane	10.80	3.6	ng	165227	4	11.40	911294	20.0
4H-Cyclopenta[def...	12.02	2.5	ng	113936	4	11.40	911294	20.0
Nonadecyl pentafl...	13.87	5.9	ng	267775	5	14.06	906770	20.0