LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097376.D
Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

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-BF072517.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	4.557	468	471	483	rBV	166511	256140	18.49%	1.804%
2	5.040	550	553	573	rBV	958795	1255569	90.62%	8.842%
3	6.110	732	735	749	rBV	1199420	1339597	96.69%	9.434%
4	6.210	749	752	764	rVB	1268344	1385487	100.00%	9.757%
5	6.439	787	791	800	rBV	658056	615949	44.46%	4.338%
6	6.592	813	817	828	rBV	994773	895478	64.63%	6.306%
7	7.004	884	887	904	rBV	771928	832271	60.07%	5.861%
8	7.722	1005	1009	1026	rVB	945157	868363	62.68%	6.115%
9	8.792	1187	1191	1195	rBV	1404703	1318326	95.15%	9.284%
10	9.198	1256	1260	1269	rVB	219622	196796	14.20%	1.386%
11	9.463	1301	1305	1313	rBV	867748	771116	55.66%	5.430%
12	9.916	1379	1382	1385	rVB	23939	19539	1.41%	0.138%
13	10.245	1435	1438	1447	rBV	530037	535123	38.62%	3.768%
14	10.386	1458	1462	1471	rBV	31064	39200	2.83%	0.276%
15	10.827	1528	1537	1540	rBV3	22366	21906	1.58%	0.154%
16	10.933	1551	1555	1558	rBV	711087	608071	43.89%	4.282%
17	10.957	1558	1559	1563	rVB	31076	19969	1.44%	0.141%
18	11.457	1642	1644	1647	rBV3	18517	20517	1.48%	0.144%
19	11.492	1647	1650	1657	rVB2	59850	67154	4.85%	0.473%
20	12.139	1756	1760	1763	rBV	82669	76883	5.55%	0.541%
21	12.280	1779	1784	1793	rBV5	8685	18390	1.33%	0.130%
22	12.363	1793	1798	1804	rVB	83441	91445	6.60%	0.644%
23	12.510	1819	1823	1827	rVB	962838	821031	59.26%	5.782%
24	12.763	1860	1866	1869	rBV3	11813	15136	1.09%	0.107%
25	13.439	1975	1981	1985	rBV5	27533	54658	3.95%	0.385%
26	13.551	1995	2000	2003	rBV	610996	592823	42.79%	4.175%
27	13.574	2003	2004	2008	rVB	42274	33395	2.41%	0.235%
28	13.945	2063	2067	2071	rBV3	13923	20019	1.44%	0.141%
29	14.045	2079	2084	2086	rBV3	14385	18481	1.33%	0.130%
30	14.074	2086	2089	2096	rVB6	20584	38665	2.79%	0.272%
31	14.268	2114	2122	2124	rBV9	12788	24877	1.80%	0.175%
32	14.462	2150	2155	2157	rBV3	42147	39509	2.85%	0.278%
33	14.545	2165	2169	2177	rBV	52574	96400	6.96%	0.679%
34	14.621	2177	2182	2187	rBV2	39133	63589	4.59%	0.448%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097376.D
Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.674	2189	2191	2197	rVB6	22618	30968	2.24%	0.218%
36	14.792	2205	2211	2214	rBV	40506	65010	4.69%	0.458%
37	14.845	2216	2220	2223	rBV	42776	43701	3.15%	0.308%
38	14.892	2223	2228	2232	rBV	435302	504254	36.40%	3.551%
39	15.086	2257	2261	2266	rVB6	25461	35409	2.56%	0.249%
40	15.274	2289	2293	2298	rBV	47860	70185	5.07%	0.494%
41	15.392	2311	2313	2318	rBV6	11794	16739	1.21%	0.118%
42	15.621	2350	2352	2357	rBV6	12955	25034	1.81%	0.176%
43	15.674	2357	2361	2366	rVB3	24501	43651	3.15%	0.307%
44	16.098	2428	2433	2435	rBV4	22002	34476	2.49%	0.243%
45	16.127	2435	2438	2441	rVV5	10353	17001	1.23%	0.120%
46	16.268	2459	2462	2465	rBV5	12648	17848	1.29%	0.126%
47	16.304	2465	2468	2474	rVB8	13066	23957	1.73%	0.169%
48	16.456	2485	2494	2498	rBV7	24253	78027	5.63%	0.549%
49	16.662	2527	2529	2535	rVB6	12995	19688	1.42%	0.139%
50	16.933	2573	2575	2579	rVB4	13498	17127	1.24%	0.121%
51	17.068	2595	2598	2600	rBV4	13217	18200	1.31%	0.128%
52	17.551	2678	2680	2688	rVB10	13179	27031	1.95%	0.190%
53	17.998	2751	2756	2757	rBV5	14044	22786	1.64%	0.160%
54	19.362	2984	2988	2993	rBV7	8975	17386	1.25%	0.122%

Sum of corrected areas: 14200350

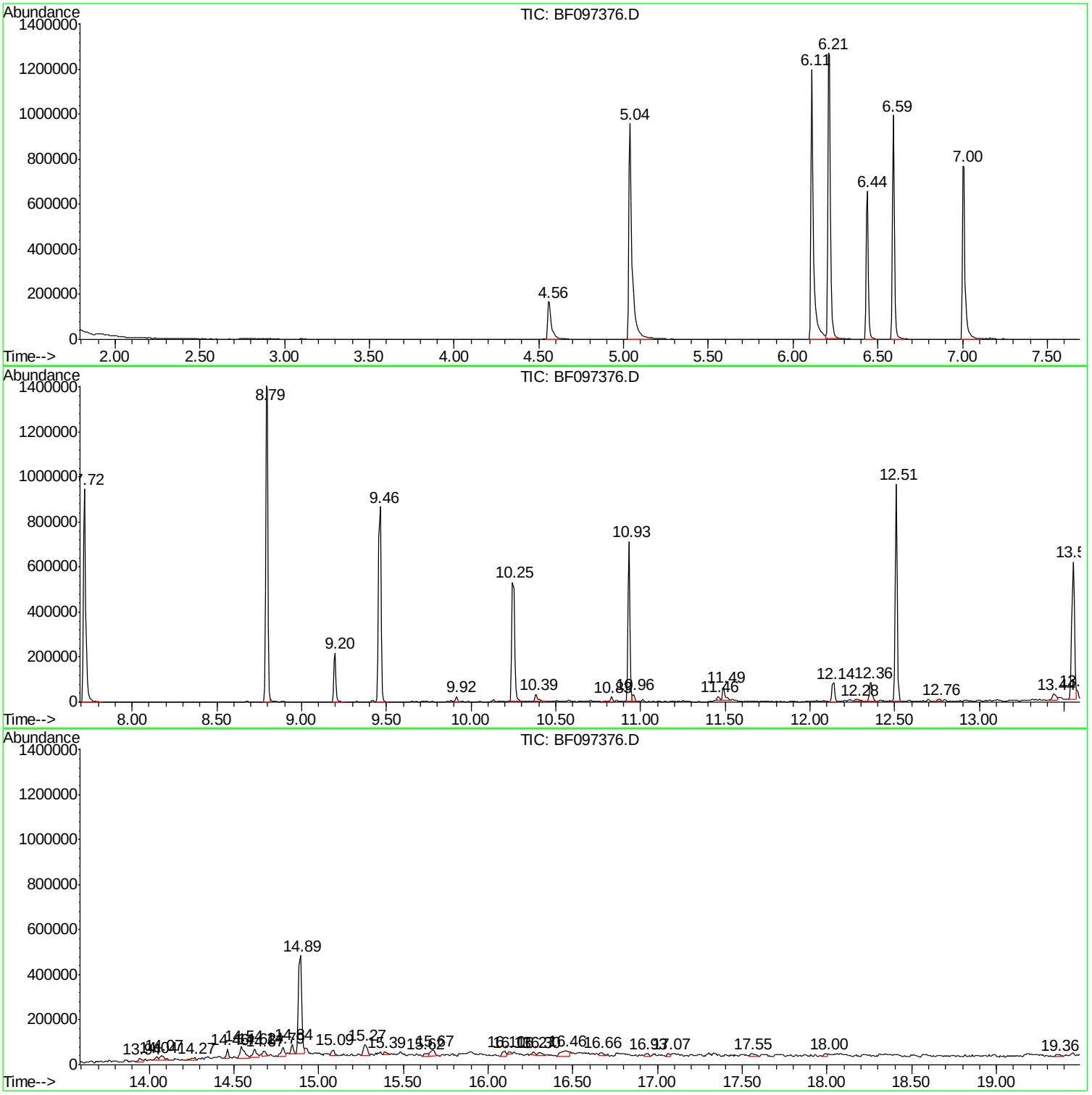
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097376.D
Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097376.D
Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

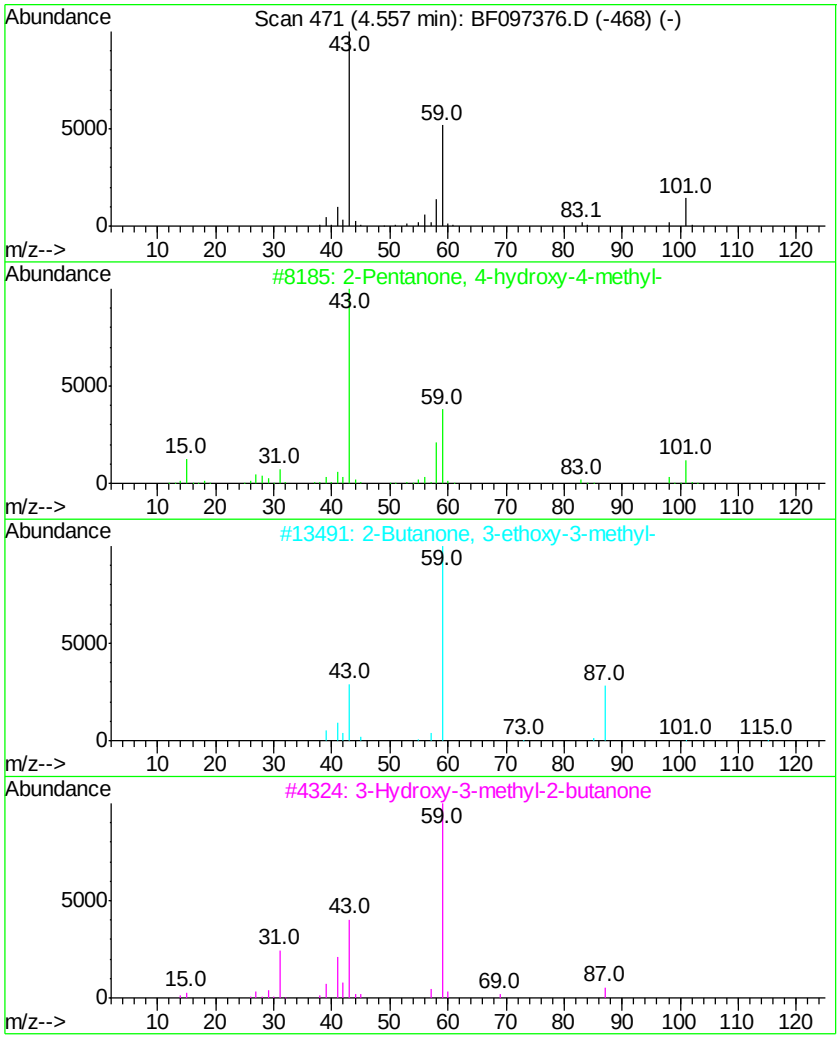
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

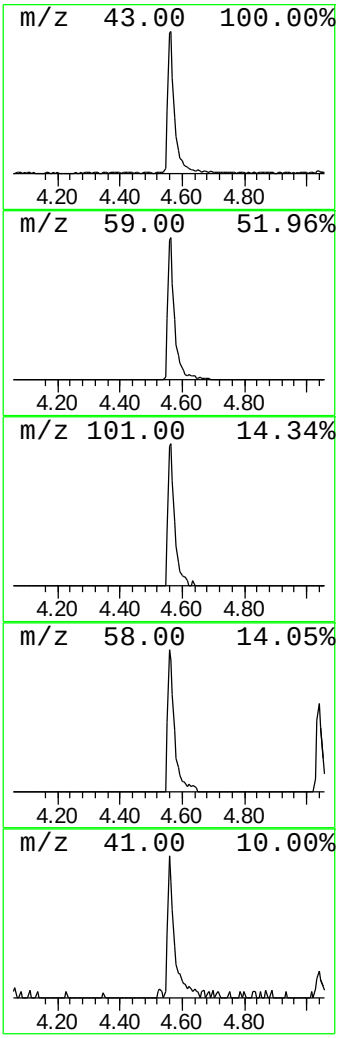
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	8.32 ng	256140	1,4-Dichlorobenzene-d4	6.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
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Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

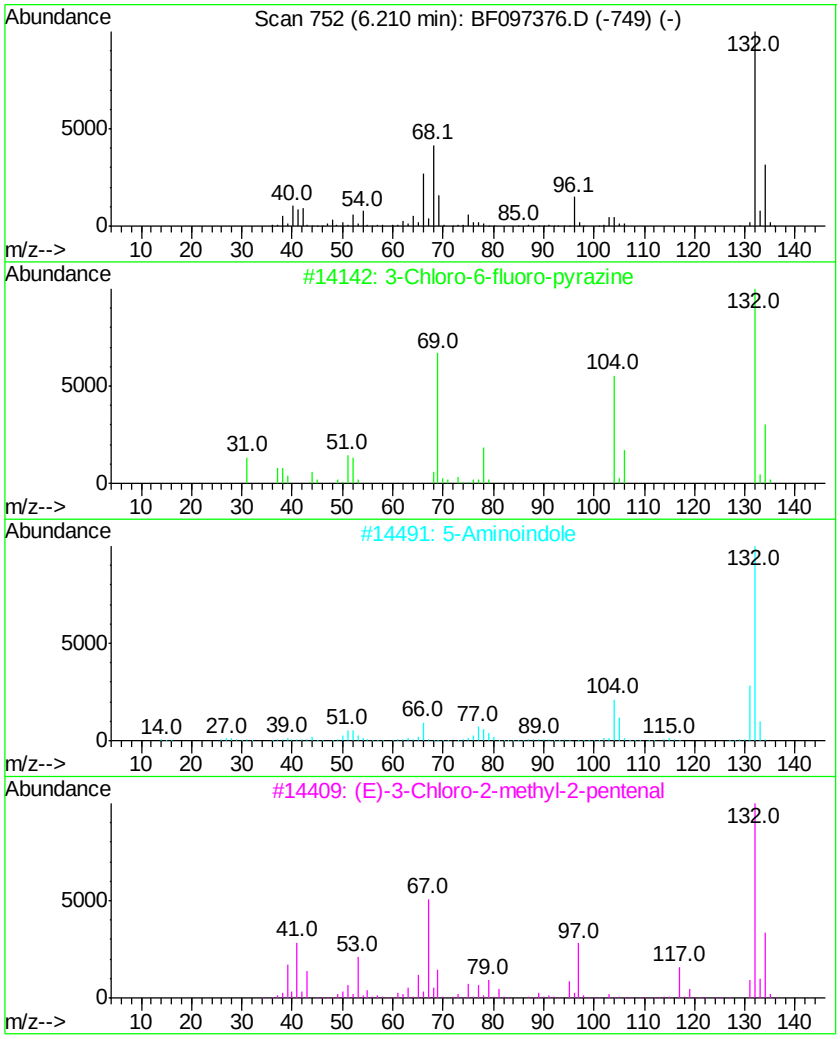
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

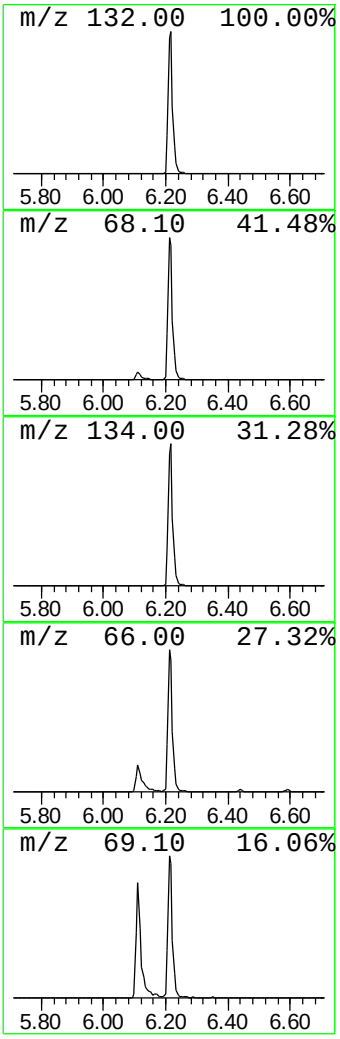
****

Peak Number 2 unknown6.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	44.99 ng	1385490	1,4-Dichlorobenzene-d4	6.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097376.D
Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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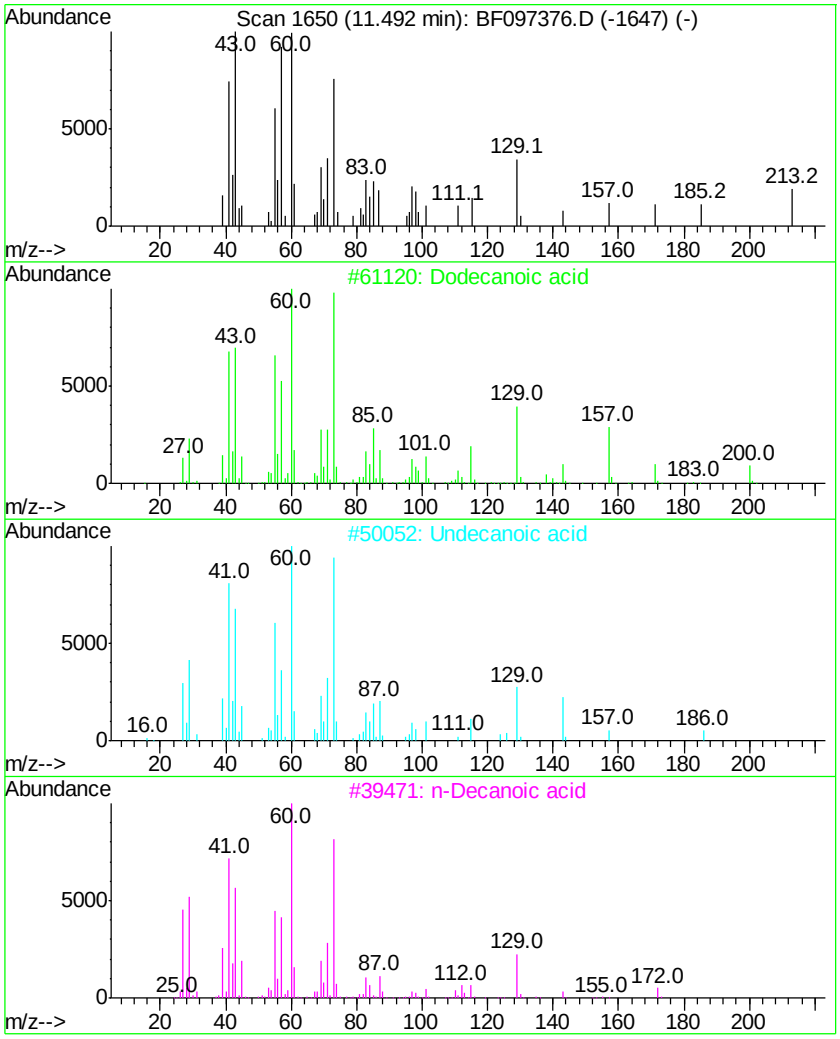
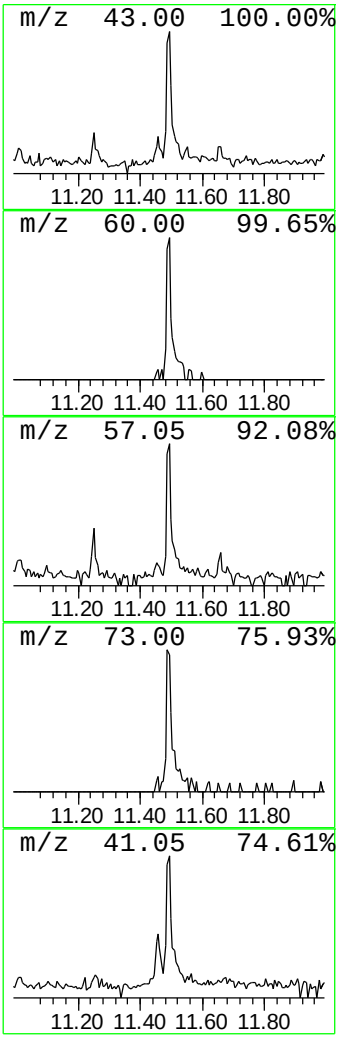
Peak Number 4 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	2.21 ng	67154	Phenanthrene-d10	10.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	58
2	Undecanoic acid	186	C11H22O2	000112-37-8	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	43
4	Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	43
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097376.D
Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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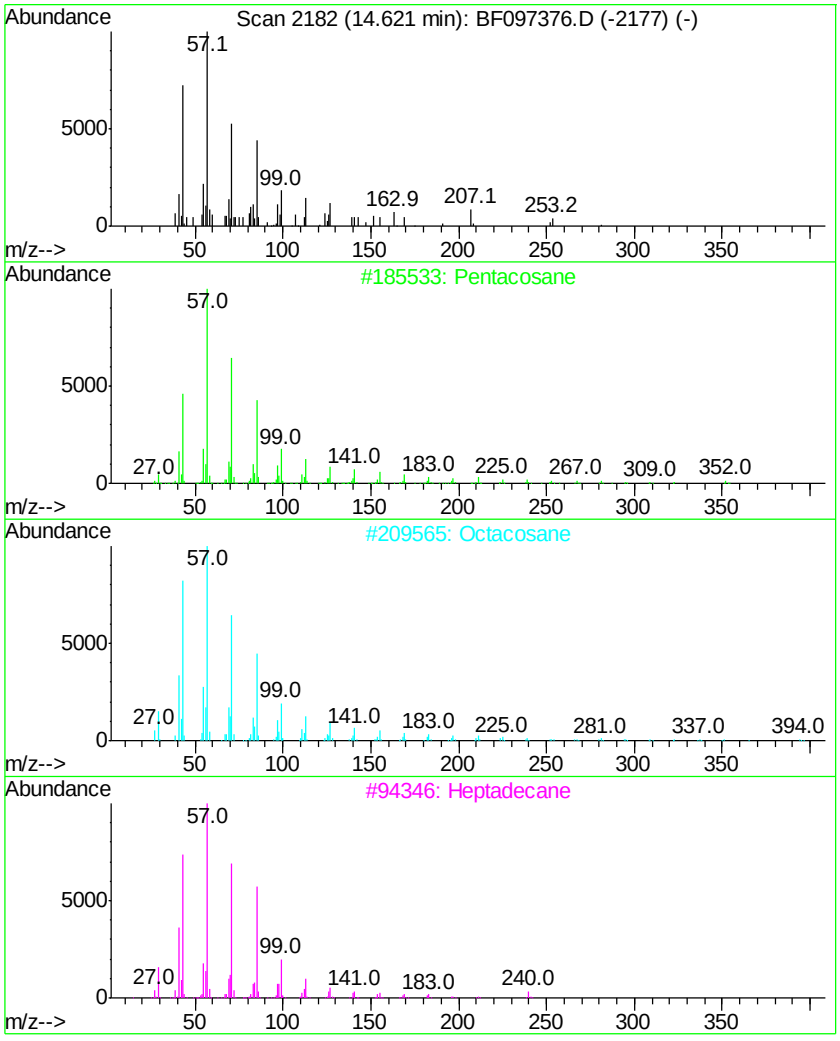
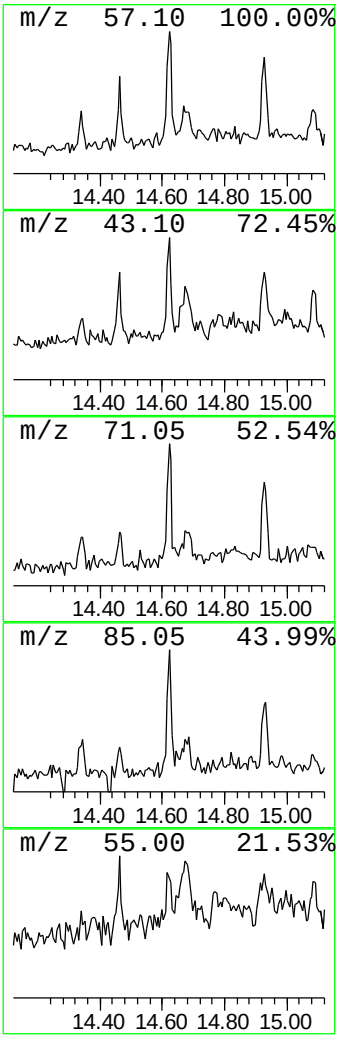
Peak Number 6 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.52 ng	63589	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Octacosane	394	C28H58	000630-02-4	86
3	Heptadecane	240	C17H36	000629-78-7	80
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5	Hentriacontane	437	C31H64	000630-04-6	74





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097376.D
Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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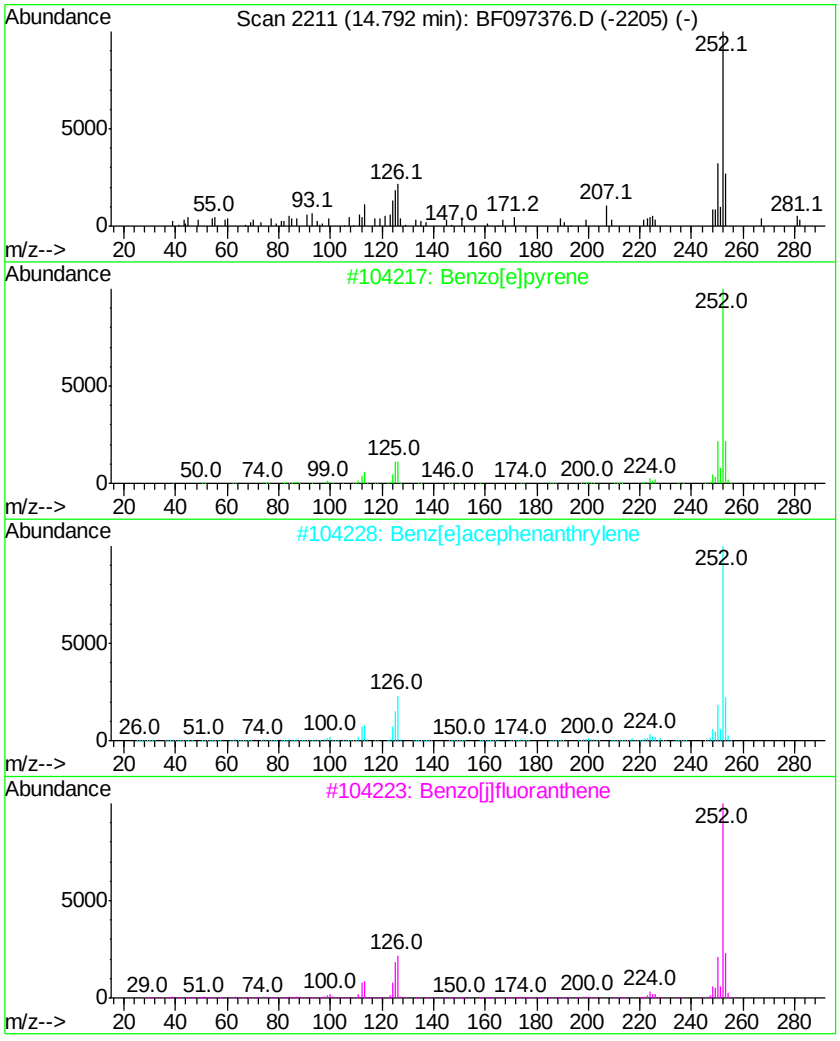
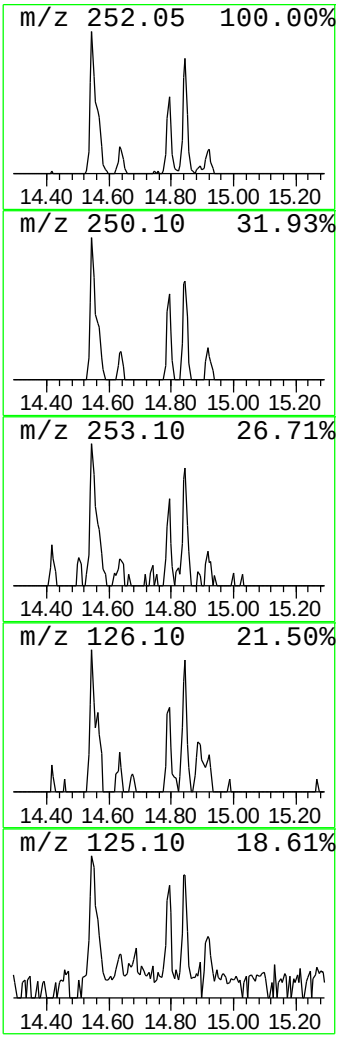
Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.58 ng	65010	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	81
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	81
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Perylene	252	C20H12	000198-55-0	81





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Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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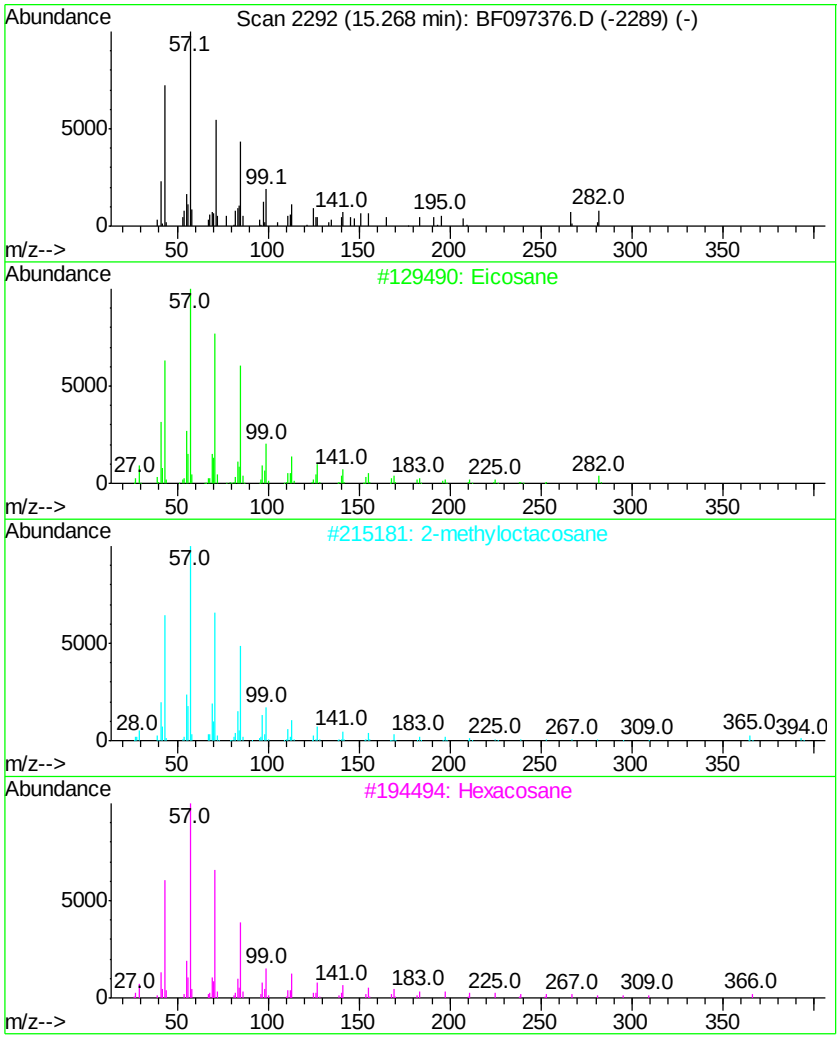
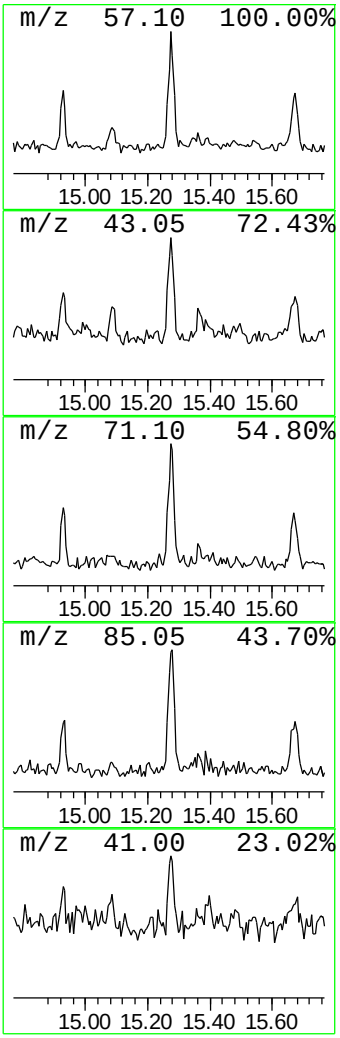
Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	2.78 ng	70185	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	80
3	Hexacosane	366	C26H54	000630-01-3	74
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	72
5	Tetracosane	338	C24H50	000646-31-1	72





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Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

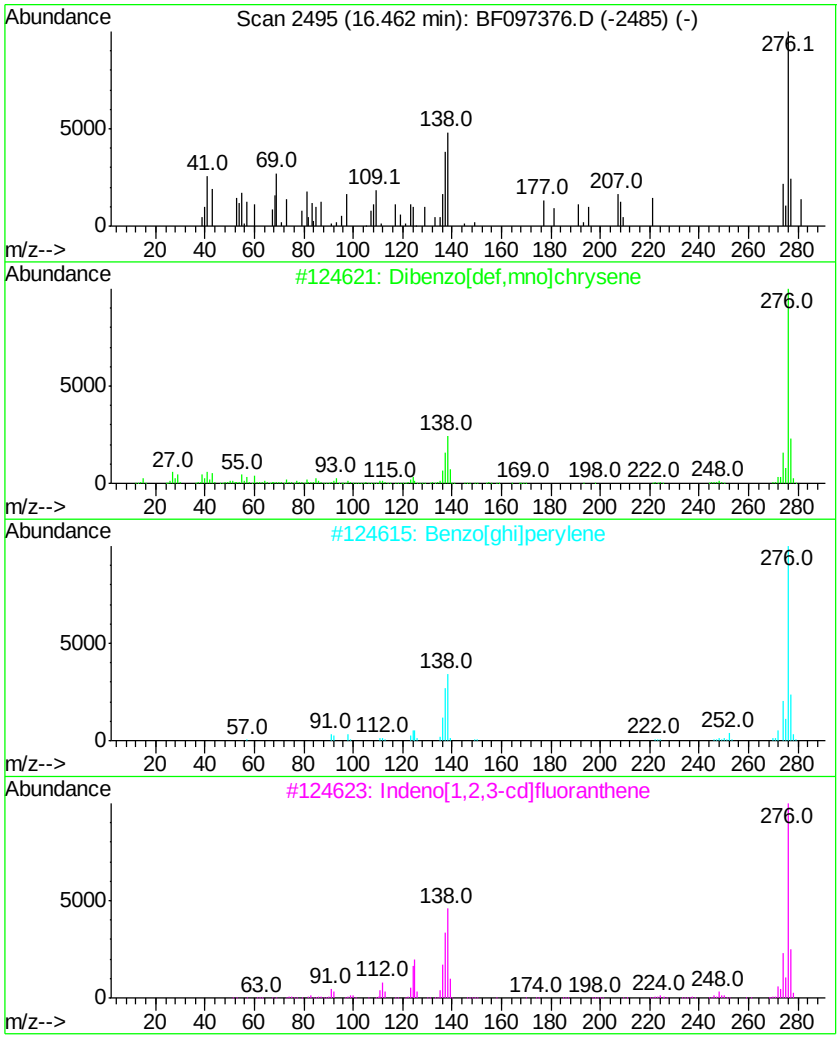
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

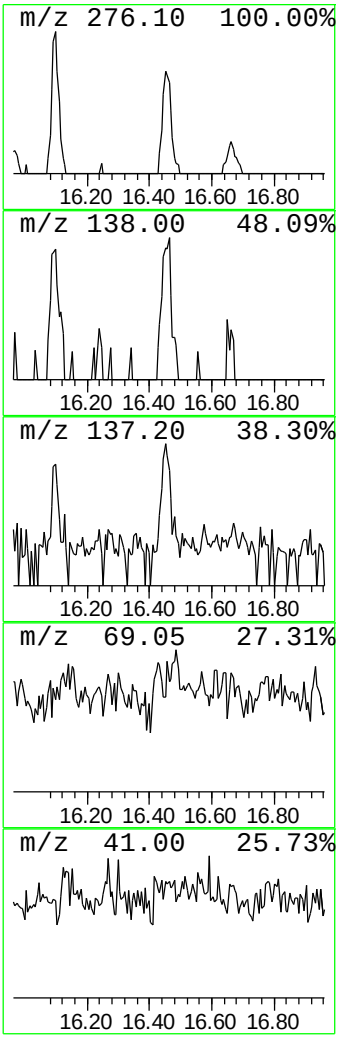
****

Peak Number 9 Dibenzo[def,mno]chrysene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	3.09 ng	78027	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	62
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	58
3	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	53
4	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	53
5	2-Amino-3-cyano-4,5-diphenylthio...	276	C17H12N2S	042160-34-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080417\
Data File : BF097376.D
Acq On : 5 Aug 2017 00:48
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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
2-Pentanone, 4-hy...	4.56	8.3	ng	256140	1	6.44	615949	20.0
unknown6.21	6.21	45.0	ng	1385490	1	6.44	615949	20.0
Dodecanoic acid	11.49	2.2	ng	67154	4	10.93	608071	20.0
Pentacosane	14.62	2.5	ng	63589	6	14.89	504254	20.0
Benzo[e]pyrene	14.79	2.6	ng	65010	6	14.89	504254	20.0
Eicosane	15.27	2.8	ng	70185	6	14.89	504254	20.0
Dibenzo[def,mno]c...	16.46	3.1	ng	78027	6	14.89	504254	20.0