LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097151.D
Acq On : 28 Jul 2017 13:43
Operator : SJ/JU
Sample : I4397-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2B-14.5-15.0-072117

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	2.657	127	131	147	rBV	170453	393040	12.77%	1.375%
2	4.640	464	468	484	rBV	181439	315629	10.25%	1.105%
3	5.092	540	545	560	rBV	2699559	3052129	99.16%	10.681%
4	6.157	720	726	736	rBV	2519683	3078049	100.00%	10.771%
5	6.263	739	744	747	rBV	3100952	2983602	96.93%	10.441%
6	6.486	778	782	793	rBV	888723	751867	24.43%	2.631%
7	6.645	804	809	812	rBV	2139197	1974362	64.14%	6.909%
8	7.057	874	879	882	rBV	1825424	1803095	58.58%	6.310%
9	7.192	898	902	912	rVB2	46761	63468	2.06%	0.222%
10	7.692	984	987	996	rBV	88469	98371	3.20%	0.344%
11	7.769	996	1000	1004	rBV	1100492	917498	29.81%	3.211%
12	8.851	1178	1184	1187	rBV	2763391	2597368	84.38%	9.089%
13	9.245	1247	1251	1256	rBV	550751	436886	14.19%	1.529%
14	9.516	1292	1297	1300	rBV	1039678	917556	29.81%	3.211%
15	9.545	1300	1302	1305	rVB	51197	37165	1.21%	0.130%
16	9.969	1371	1374	1377	rVB	56776	44407	1.44%	0.155%
17	10.057	1382	1389	1395	rVB2	32679	40553	1.32%	0.142%
18	10.298	1426	1430	1437	rBV	1329283	1375867	44.70%	4.815%
19	10.439	1450	1454	1463	rVB	70352	79915	2.60%	0.280%
20	10.886	1525	1530	1532	rBV	69735	60864	1.98%	0.213%
21	10.986	1543	1547	1549	rBV	831258	707441	22.98%	2.476%
22	11.010	1549	1551	1555	rVB	477606	367118	11.93%	1.285%
23	11.063	1555	1560	1564	rVB	124476	102579	3.33%	0.359%
24	11.221	1583	1587	1593	rBV2	33527	37176	1.21%	0.130%
25	11.486	1629	1632	1635	rBV	41756	33713	1.10%	0.118%
26	11.516	1635	1637	1639	rBV	51584	39707	1.29%	0.139%
27	11.598	1648	1651	1653	rBV	67329	59426	1.93%	0.208%
28	12.192	1748	1752	1756	rBV	623921	519287	16.87%	1.817%
29	12.333	1772	1776	1780	rBV3	27011	40404	1.31%	0.141%
30	12.416	1785	1790	1794	rBV	558156	532067	17.29%	1.862%
31	12.574	1812	1817	1820	rVB	1567618	1555365	50.53%	5.443%
32	12.639	1823	1828	1832	rBV2	25818	46024	1.50%	0.161%
33	12.751	1844	1847	1850	rVB	57773	52939	1.72%	0.185%
34	12.851	1861	1864	1866	rBV	50128	49194	1.60%	0.172%

LSC Area Percent Report

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Data File : BF097151.D
Acq On : 28 Jul 2017 13:43
Operator : SJ/JU
Sample : I4397-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2B-14.5-15.0-072117

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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	13.121	1906	1910	1912	rBV	63865	65047	2.11%	0.228%
36	13.257	1931	1933	1938	rVB	35645	33246	1.08%	0.116%
37	13.363	1947	1951	1953	rBV	53788	48369	1.57%	0.169%
38	13.463	1965	1968	1969	rBV	50478	40639	1.32%	0.142%
39	13.486	1969	1972	1976	rVB2	82297	105994	3.44%	0.371%
40	13.610	1985	1993	1996	rBV2	767995	975907	31.71%	3.415%
41	13.633	1996	1997	2001	rVB	234420	192034	6.24%	0.672%
42	13.715	2008	2011	2013	rBV	46590	36813	1.20%	0.129%
43	13.998	2057	2059	2062	rVB2	34929	32082	1.04%	0.112%
44	14.468	2136	2139	2141	rBV2	35870	36924	1.20%	0.129%
45	14.604	2158	2162	2170	rBV	281885	472919	15.36%	1.655%
46	14.692	2175	2177	2180	rVB	61105	58759	1.91%	0.206%
47	14.857	2202	2205	2211	rVB	128925	138558	4.50%	0.485%
48	14.909	2211	2214	2219	rBV	180686	196964	6.40%	0.689%
49	14.962	2219	2223	2226	rBV	467479	518403	16.84%	1.814%
50	15.680	2343	2345	2349	rBV5	25667	38279	1.24%	0.134%
51	16.027	2399	2404	2407	rBV5	33725	67059	2.18%	0.235%
52	16.180	2427	2430	2437	rVB2	82536	140816	4.57%	0.493%
53	16.545	2488	2492	2502	rVB	66396	133344	4.33%	0.467%
54	17.027	2572	2574	2577	rBV3	33195	48805	1.59%	0.171%
55	17.862	2714	2716	2721	rBV6	18870	31230	1.01%	0.109%

Sum of corrected areas: 28576322

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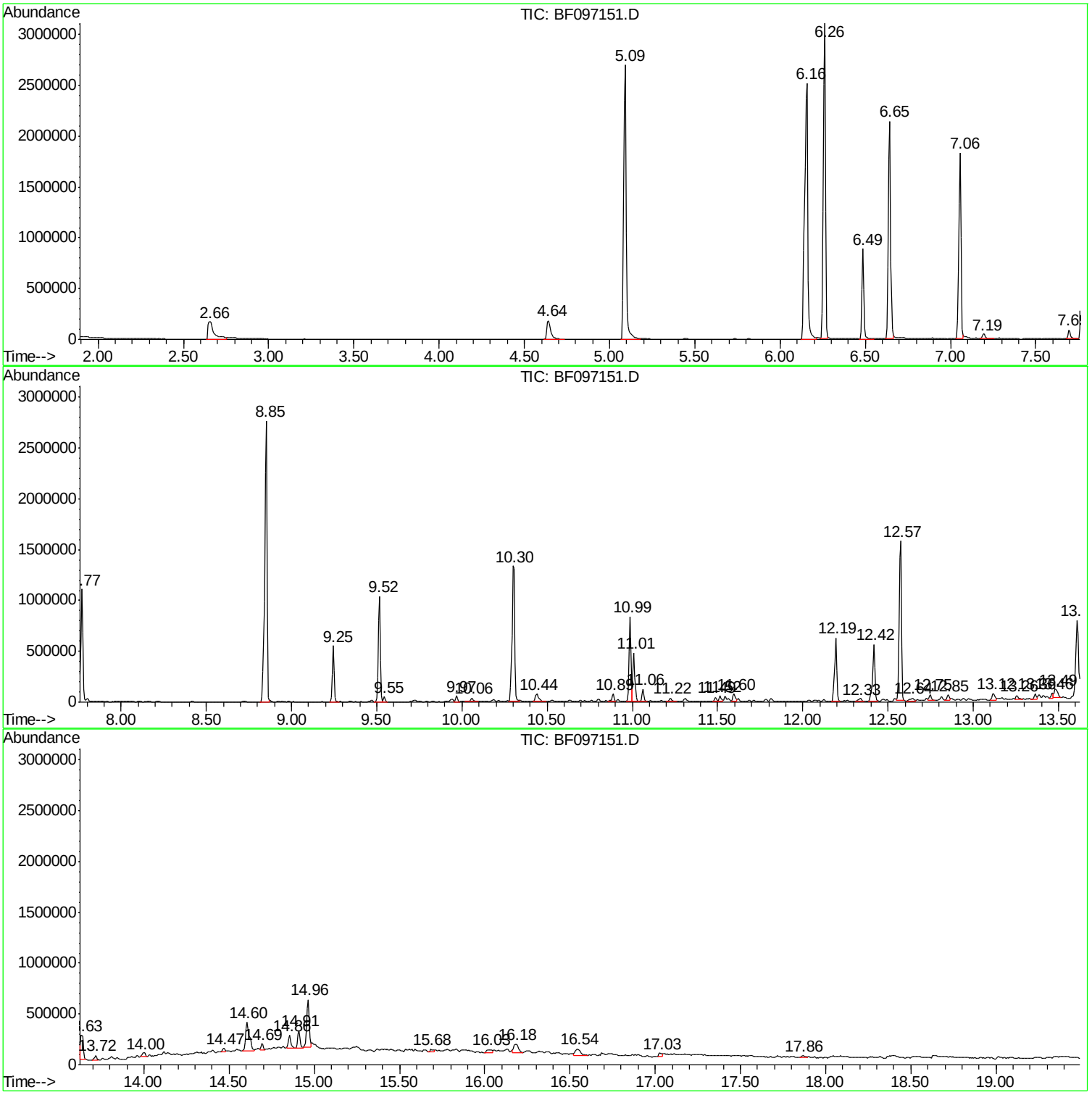
BNA_F
ClientSampleId :
T-2B-14.5-15.0-072117

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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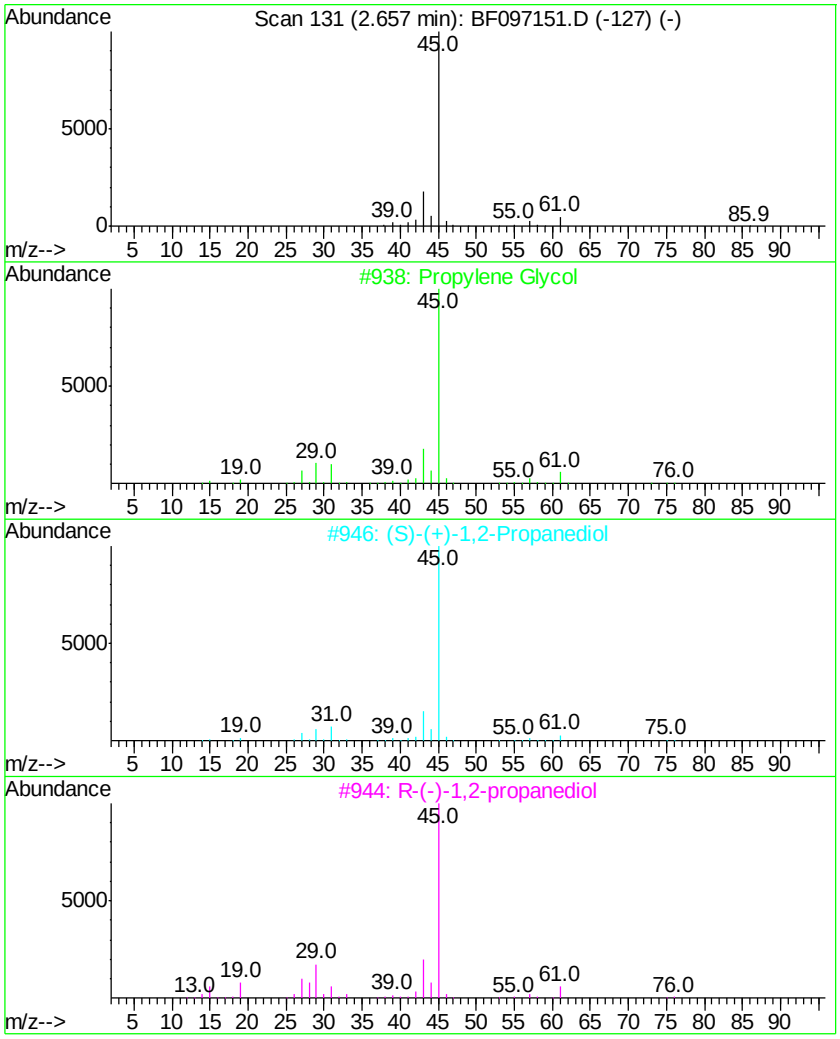
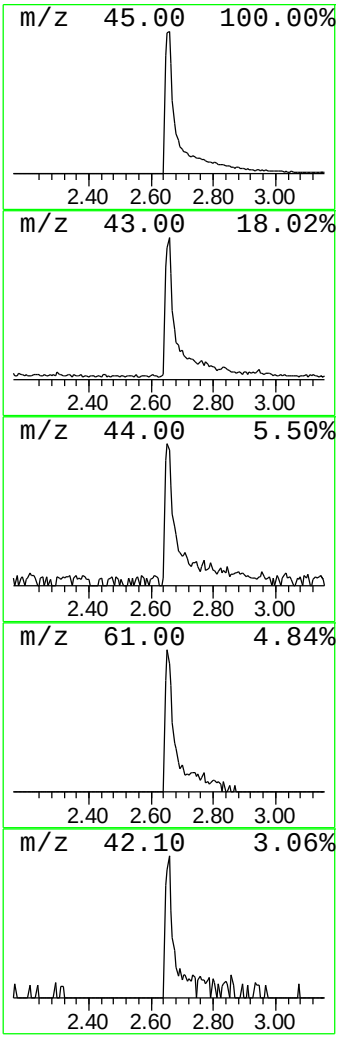
Peak Number 1 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.66	10.46 ng	393040	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	74
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9





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Operator : SJ/JU
Sample : I4397-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2B-14.5-15.0-072117

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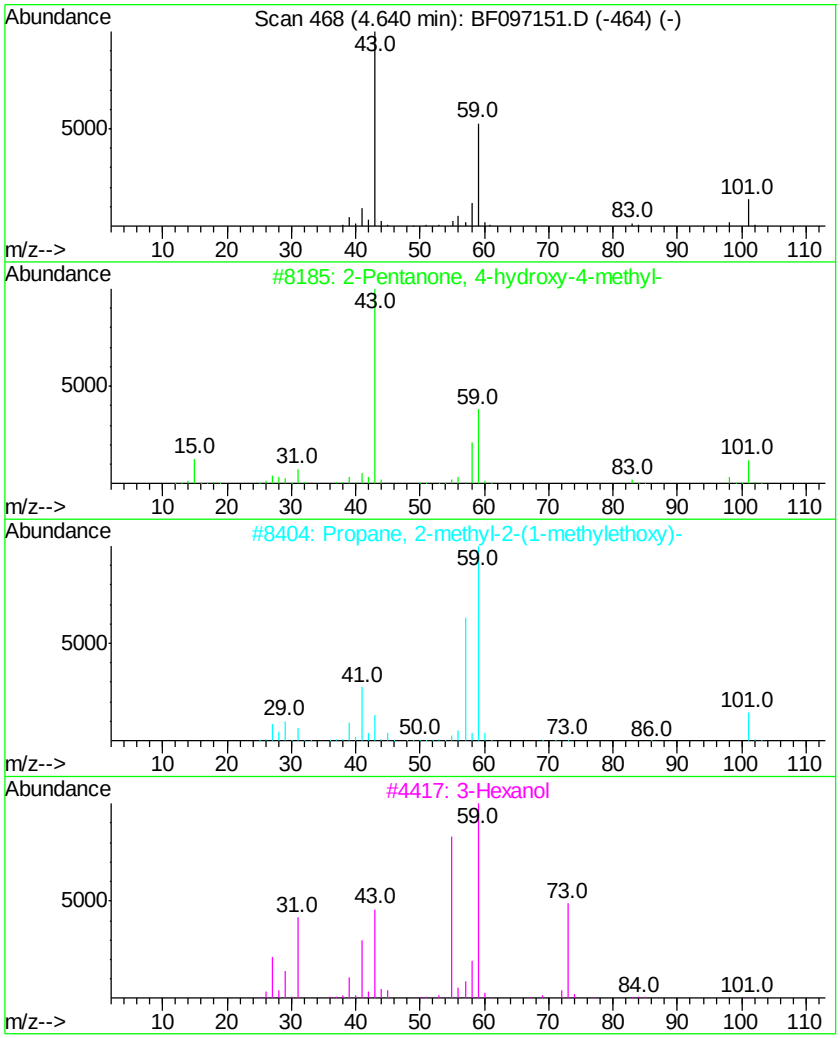
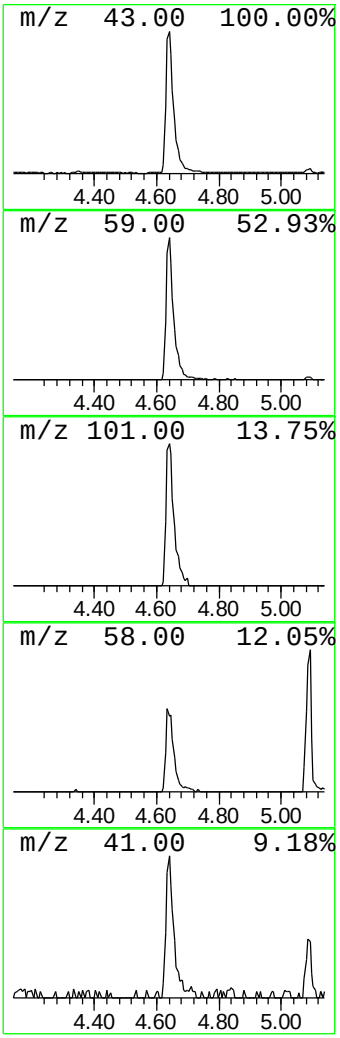
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	8.40 ng	315629	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





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Sample : I4397-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-2B-14.5-15.0-072117

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
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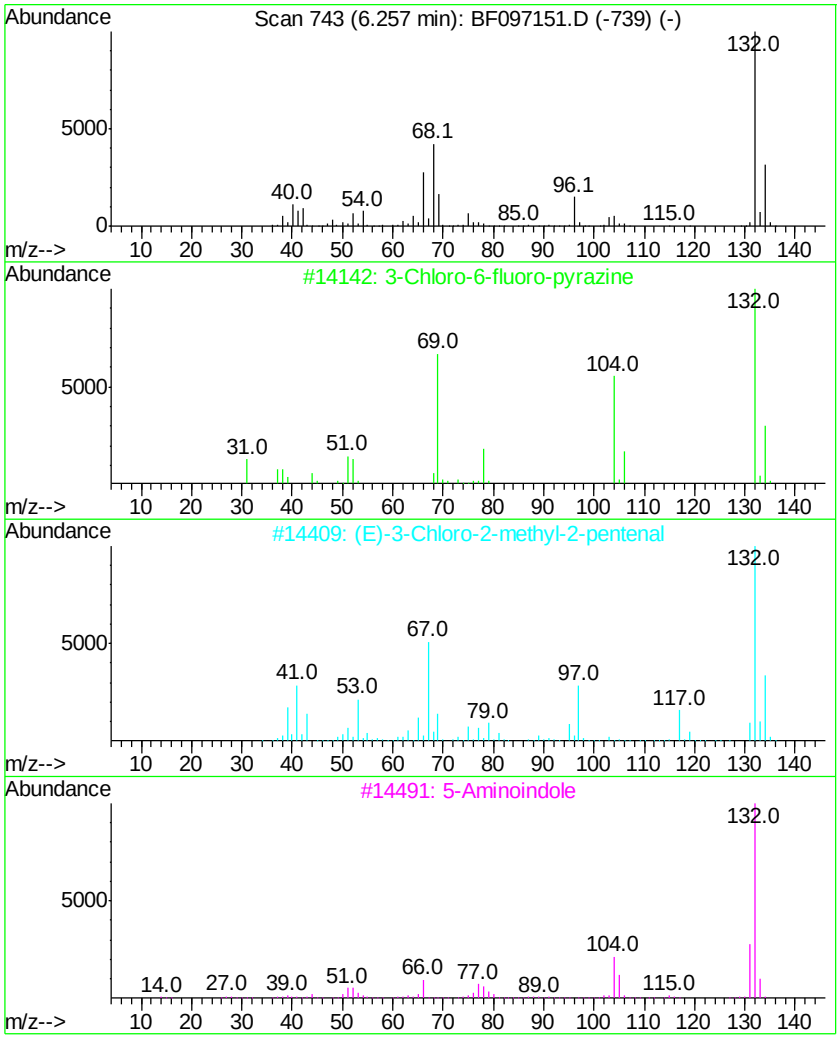
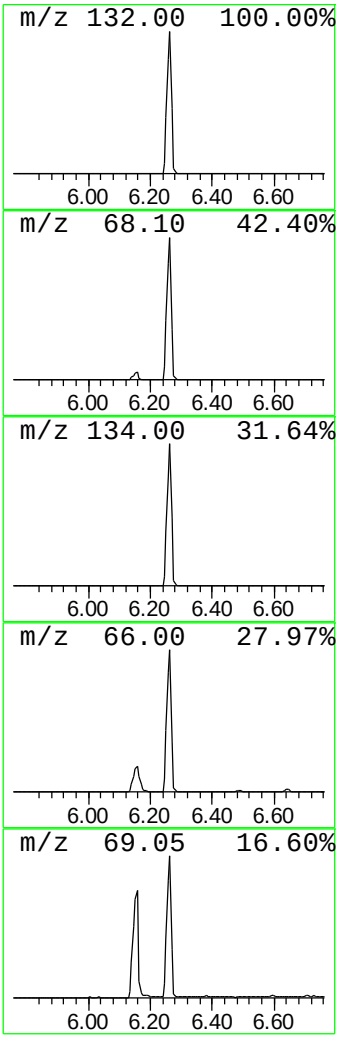
Peak Number 3 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	79.37 ng	2983600	1,4-Dichlorobenzene-d4	6.49

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Instrument : BNA_F
ClientSampleId : T-2B-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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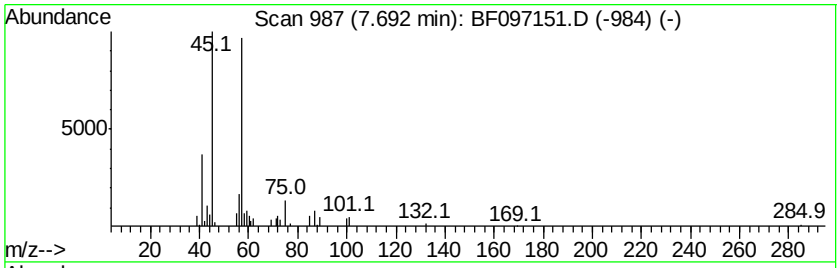
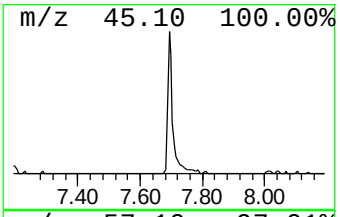
****

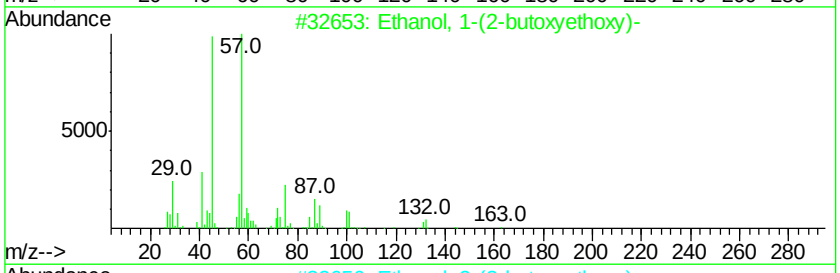
Peak Number 5 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 10

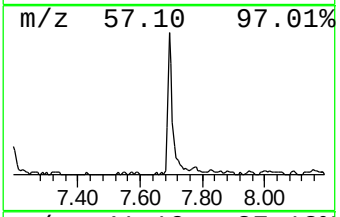
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	2.14 ng	98371	Naphthalene-d8	7.77

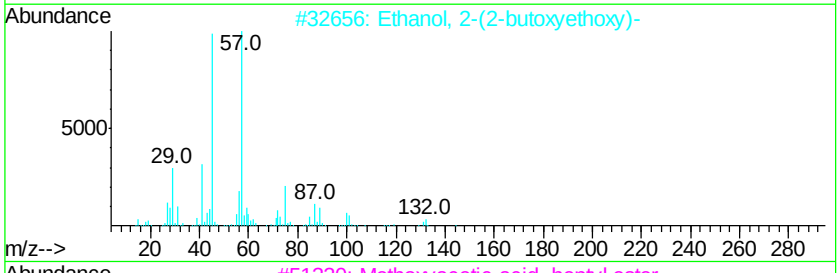
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
3	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
4	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47
5	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	45

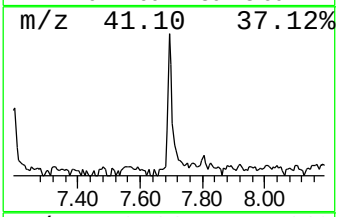


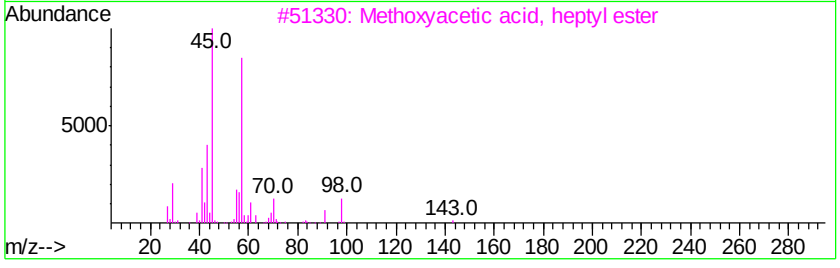


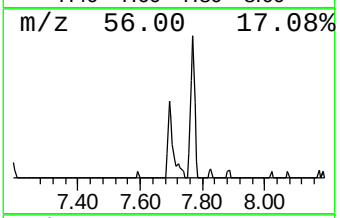


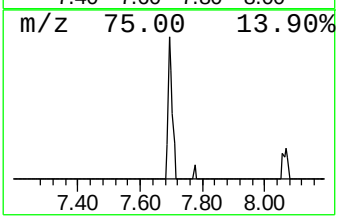












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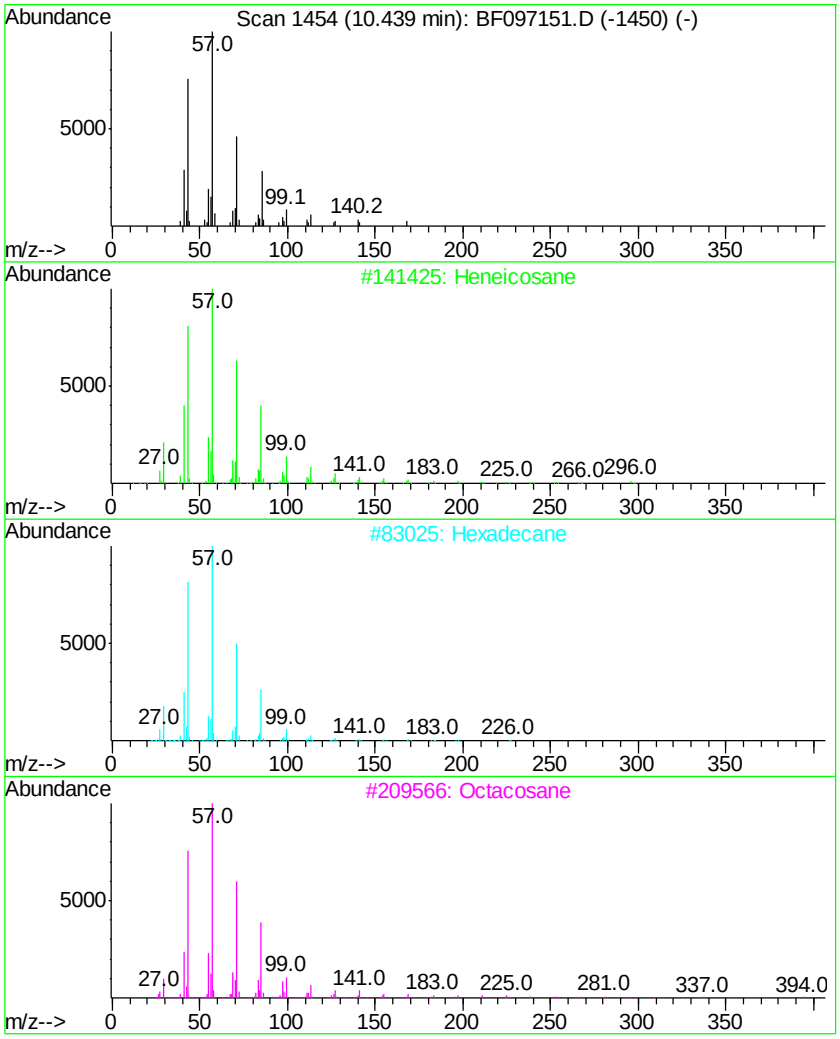
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

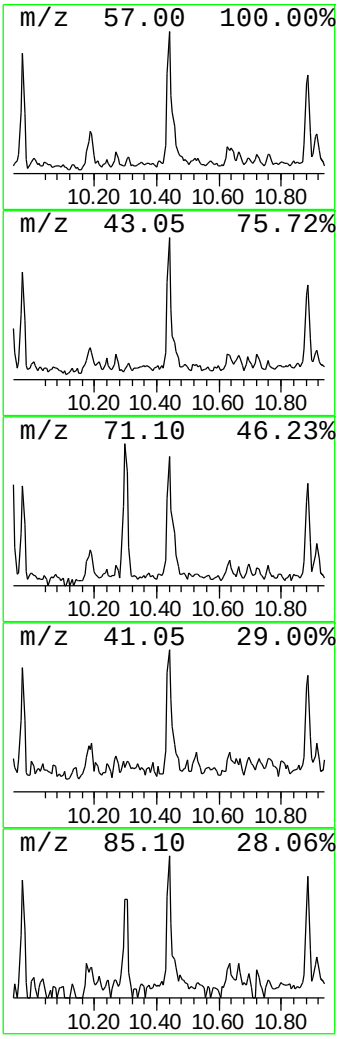
****

Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.26 ng	79915	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexadecane	226	C16H34	000544-76-3	87
3	Octacosane	394	C28H58	000630-02-4	86
4	Octadecane	254	C18H38	000593-45-3	72
5	Eicosane	282	C20H42	000112-95-8	72





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Instrument : BNA_F
ClientSampleId : T-2B-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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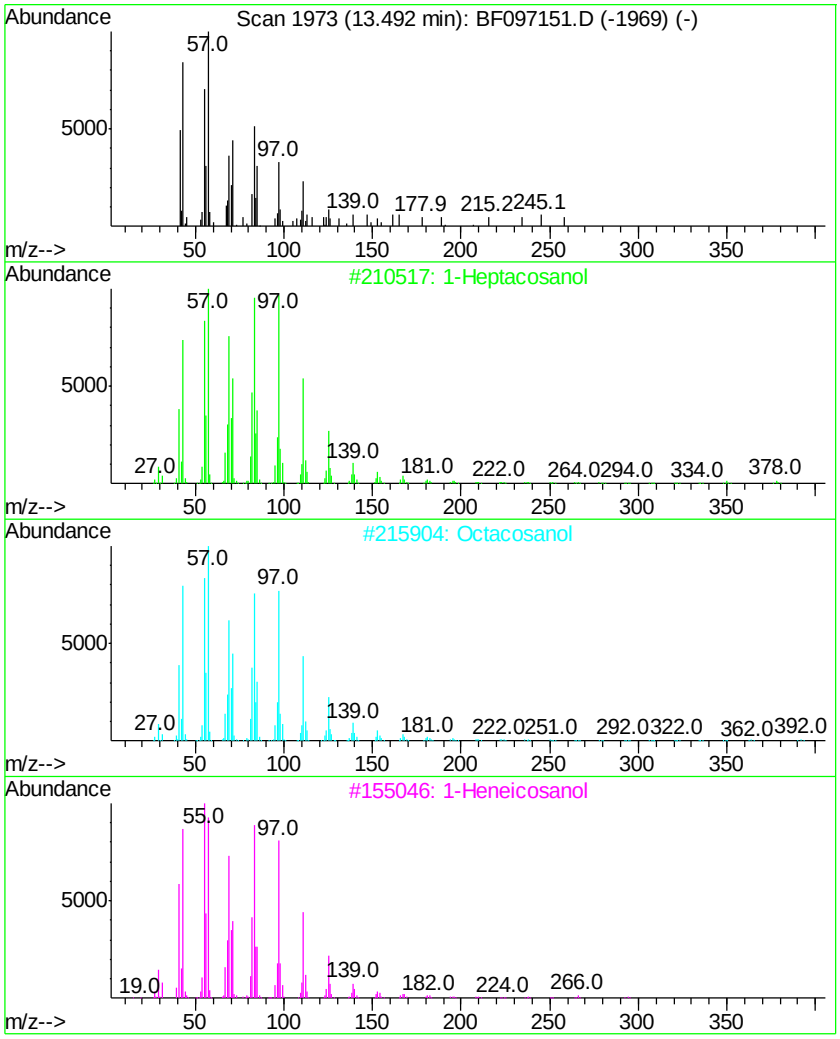
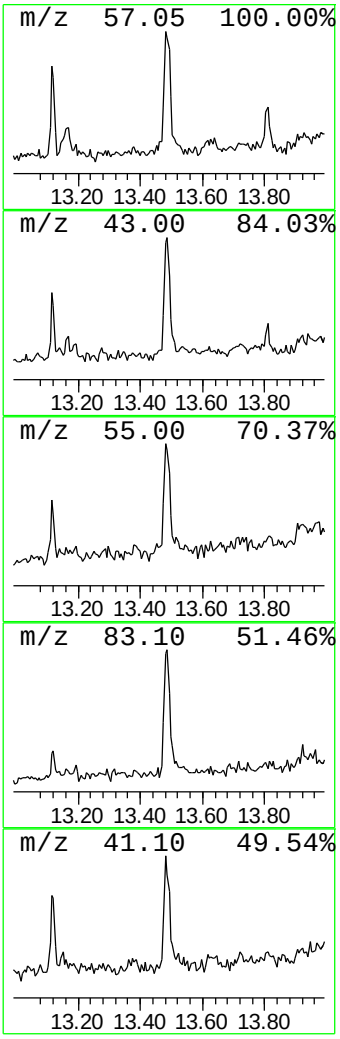
Peak Number 7 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.17 ng	105994	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	Octacosanol	410	C28H58O	000557-61-9	86
3	1-Heneicosanol	312	C21H44O	015594-90-8	83
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	83
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	83





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Data File : BF097151.D
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Sample : I4397-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2B-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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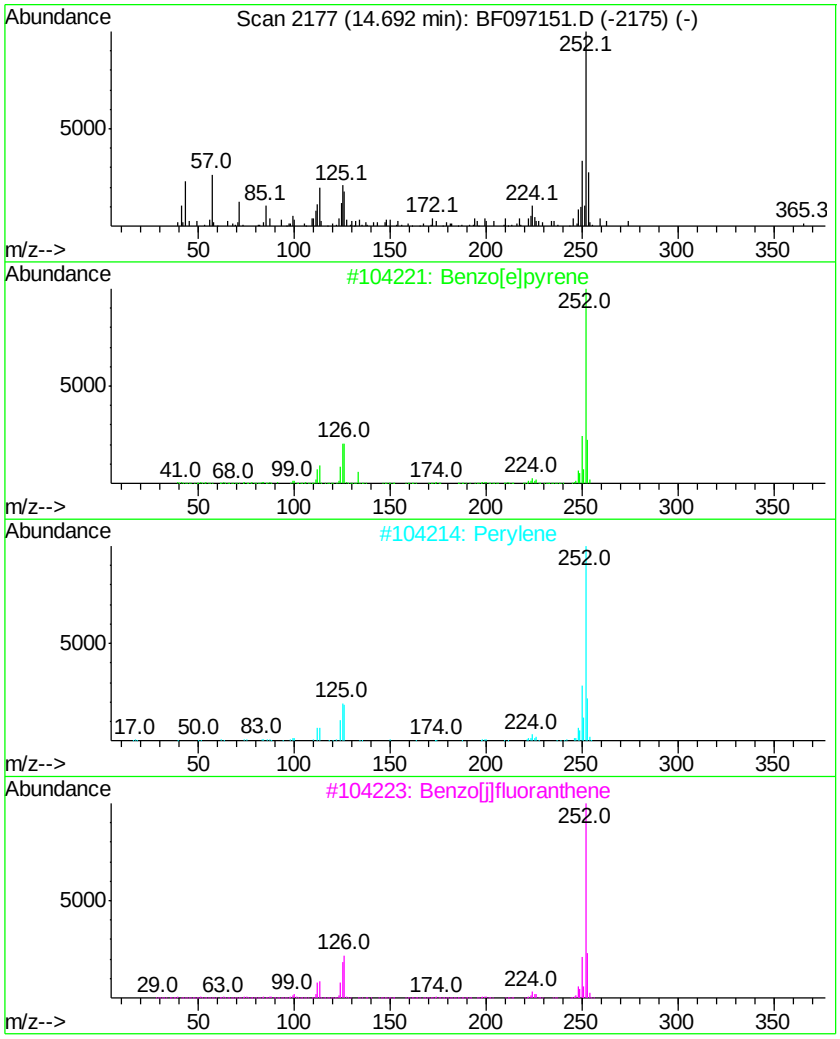
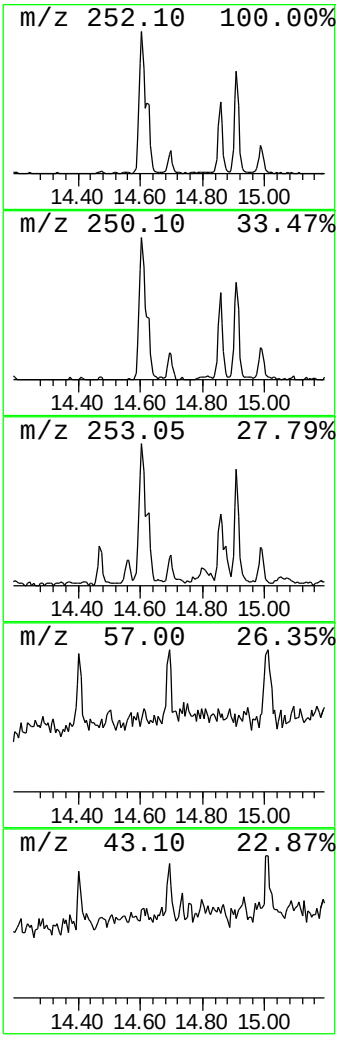
Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.27 ng	58759	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	92
2	Perylene	252	C20H12	000198-55-0	92
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	70
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	70
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097151.D
Acq On : 28 Jul 2017 13:43
Operator : SJ/JU
Sample : I4397-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2B-14.5-15.0-072117

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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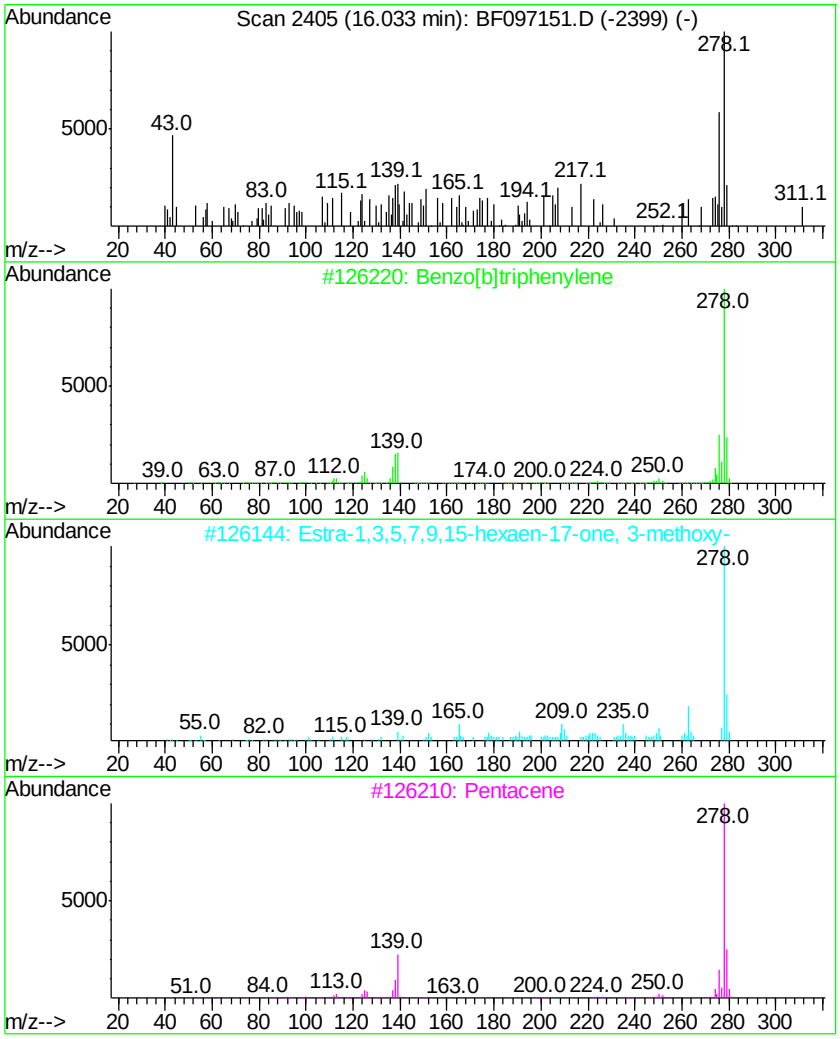
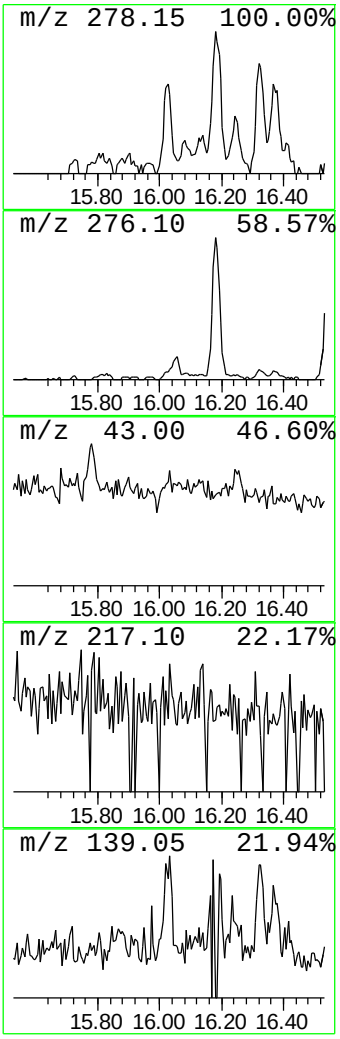
Peak Number 10 Benzo[b]triphenylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.59 ng	67059	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]triphenylene	278	C22H14	000215-58-7	55
2	Estra-1,3,5,7,9,15-hexaen-17-one...	278	C19H18O2	056588-53-5	45
3	Pentacene	278	C22H14	000135-48-8	45
4	Quinoxaline, 6-(3-nitrobenzylide...	278	C15H10N4O2	302800-55-1	43
5	Naphtho[1,2-a]anthracene	278	C22H14	000195-06-2	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097151.D
Acq On : 28 Jul 2017 13:43
Operator : SJ/JU
Sample : I4397-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2B-14.5-15.0-072117

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
Propylene Glycol	2.66	10.5	ng	393040	1	6.49	751867	20.0
2-Pentanone, 4-hy...	4.64	8.4	ng	315629	1	6.49	751867	20.0
unknown6.26	6.26	79.4	ng	2983600	1	6.49	751867	20.0
Ethanol, 1-(2-but...	7.69	2.1	ng	98371	2	7.77	917498	20.0
Heneicosane	10.44	2.3	ng	79915	4	10.99	707441	20.0
1-Heptacosanol	13.49	2.2	ng	105994	5	13.61	975907	20.0
Benzo[e]pyrene	14.69	2.3	ng	58759	6	14.96	518403	20.0
Benzo[b]triphenylene	16.03	2.6	ng	67059	6	14.96	518403	20.0