LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097978.D
Acq On : 23 Aug 2017 2:45
Operator : SJ/JU
Sample : I4910-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7-8

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-BF081517.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	3.145	177	180	193	rBV	67708	137865	3.52%	0.423%
2	4.957	484	488	499	rVB	321895	477088	12.19%	1.463%
3	5.369	552	558	561	rBV	3255045	3697624	94.46%	11.339%
4	6.392	726	732	735	rBV	3364490	3914579	100.00%	12.005%
5	6.522	749	754	757	rBV	3462329	3652818	93.31%	11.202%
6	6.751	789	793	796	rBV	1039733	867107	22.15%	2.659%
7	6.910	815	820	823	rBV	2856898	2877107	73.50%	8.823%
8	7.316	883	889	892	rBV	2353009	2468331	63.05%	7.570%
9	7.404	900	904	912	rVB2	37930	53225	1.36%	0.163%
10	8.033	1006	1011	1013	rBV	1204855	1107746	28.30%	3.397%
11	8.051	1013	1014	1019	rVB	122140	77762	1.99%	0.238%
12	9.110	1188	1194	1197	rBV	3734358	3714853	94.90%	11.392%
13	9.504	1257	1261	1264	rBV	657147	544904	13.92%	1.671%
14	9.786	1302	1309	1312	rBV	1106756	1063836	27.18%	3.262%
15	10.221	1380	1383	1386	rVB	57781	43606	1.11%	0.134%
16	10.327	1398	1401	1408	rVB	49282	41815	1.07%	0.128%
17	10.568	1437	1442	1446	rBV	1620893	1703017	43.50%	5.223%
18	10.692	1460	1463	1471	rBV	81002	87945	2.25%	0.270%
19	11.139	1536	1539	1541	rBV	54155	45475	1.16%	0.139%
20	11.262	1557	1560	1563	rBV	1002782	920691	23.52%	2.823%
21	11.286	1563	1564	1567	rVB	167187	108226	2.76%	0.332%
22	11.339	1567	1573	1576	rBV	53582	58377	1.49%	0.179%
23	11.792	1648	1650	1654	rBV2	51770	54701	1.40%	0.168%
24	11.874	1661	1664	1667	rBV2	51792	57066	1.46%	0.175%
25	12.315	1736	1739	1742	rBV	173173	184222	4.71%	0.565%
26	12.474	1763	1766	1769	rVB	147389	125786	3.21%	0.386%
27	12.704	1802	1805	1807	rVB	123385	111142	2.84%	0.341%
28	12.857	1826	1831	1834	rBV	2432223	2503467	63.95%	7.677%
29	13.751	1980	1983	1990	rVB	164783	175982	4.50%	0.540%
30	13.898	2004	2008	2011	rBV	894980	871844	22.27%	2.674%
31	14.909	2178	2180	2188	rVB	43382	82321	2.10%	0.252%
32	15.321	2245	2250	2254	rBV	551696	652541	16.67%	2.001%
33	15.780	2325	2328	2331	rVB3	38522	46205	1.18%	0.142%
34	16.256	2404	2409	2416	rVB4	41507	79508	2.03%	0.244%

LSC Area Percent Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7-8

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

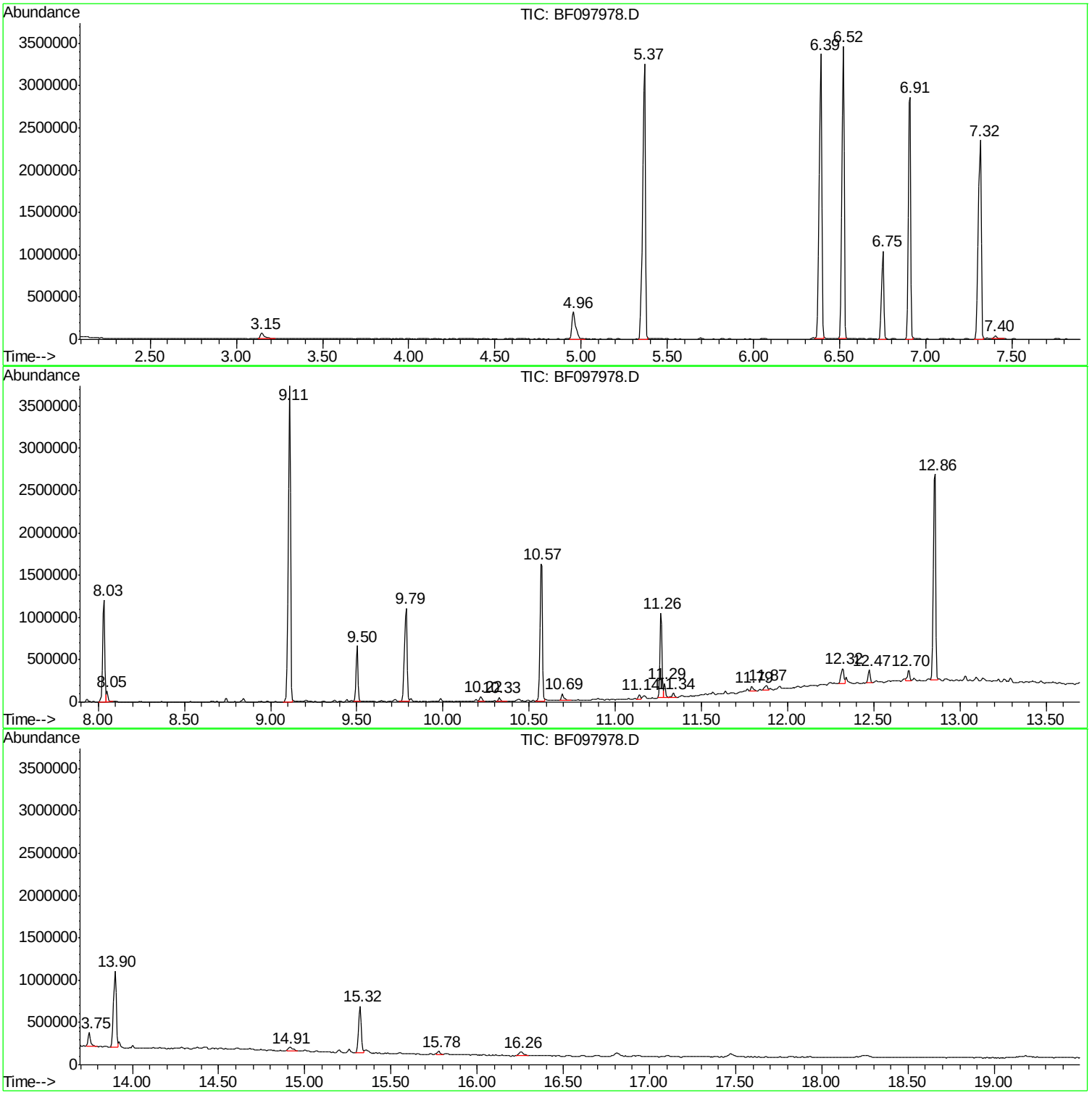
Sum of corrected areas: 32608782

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097978.D
Acq On : 23 Aug 2017 2:45
Operator : SJ/JU
Sample : I4910-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-7-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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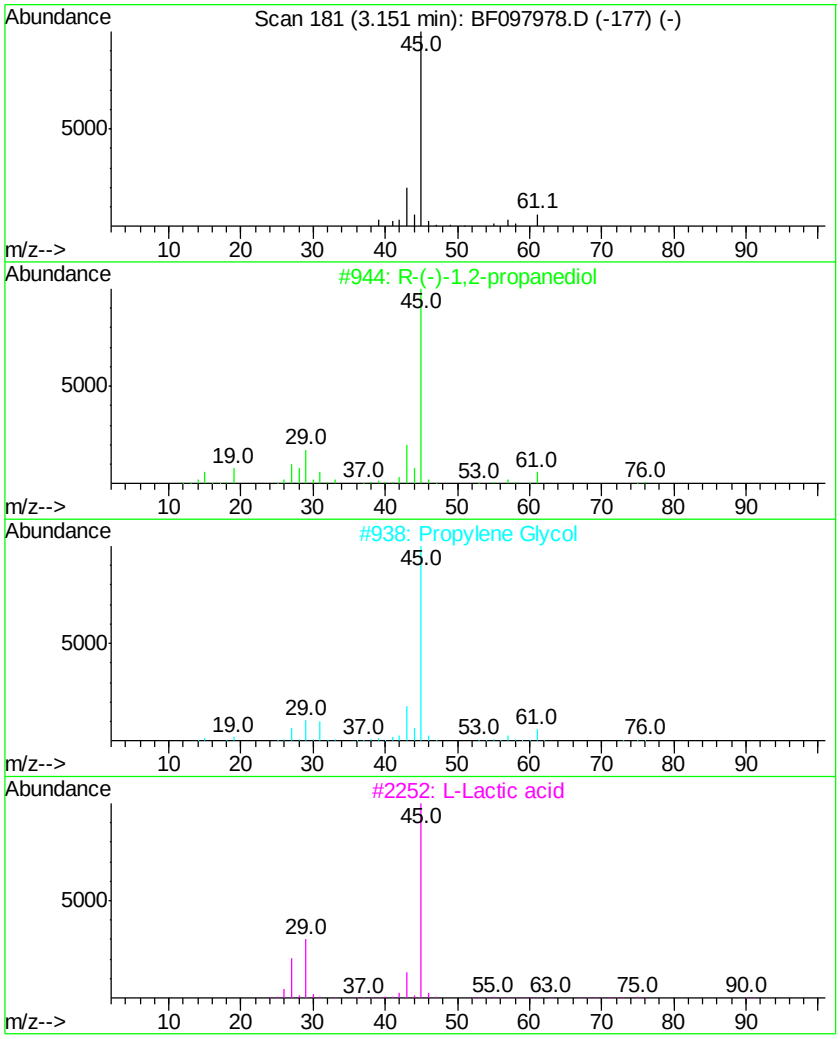
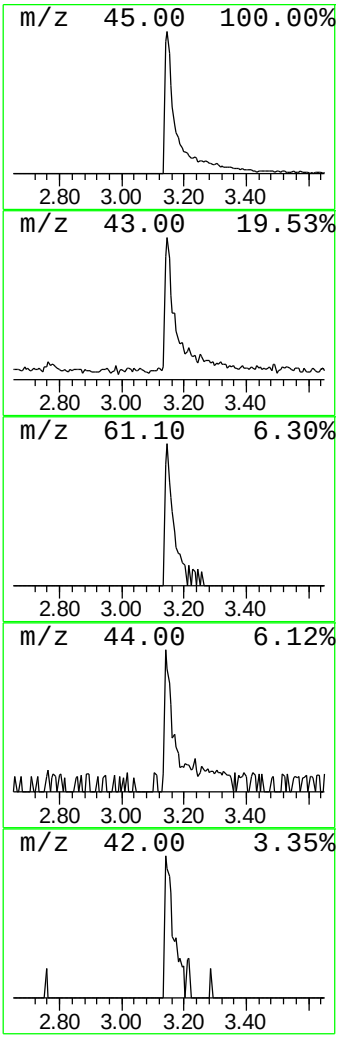
Peak Number 1 unknown3.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	3.18 ng	137865	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	40
3	L-Lactic acid	90	C3H6O3	000079-33-4	9
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5	Formamide	45	CH3NO	000075-12-7	7





Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097978.D
Acq On : 23 Aug 2017 2:45
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Sample : I4910-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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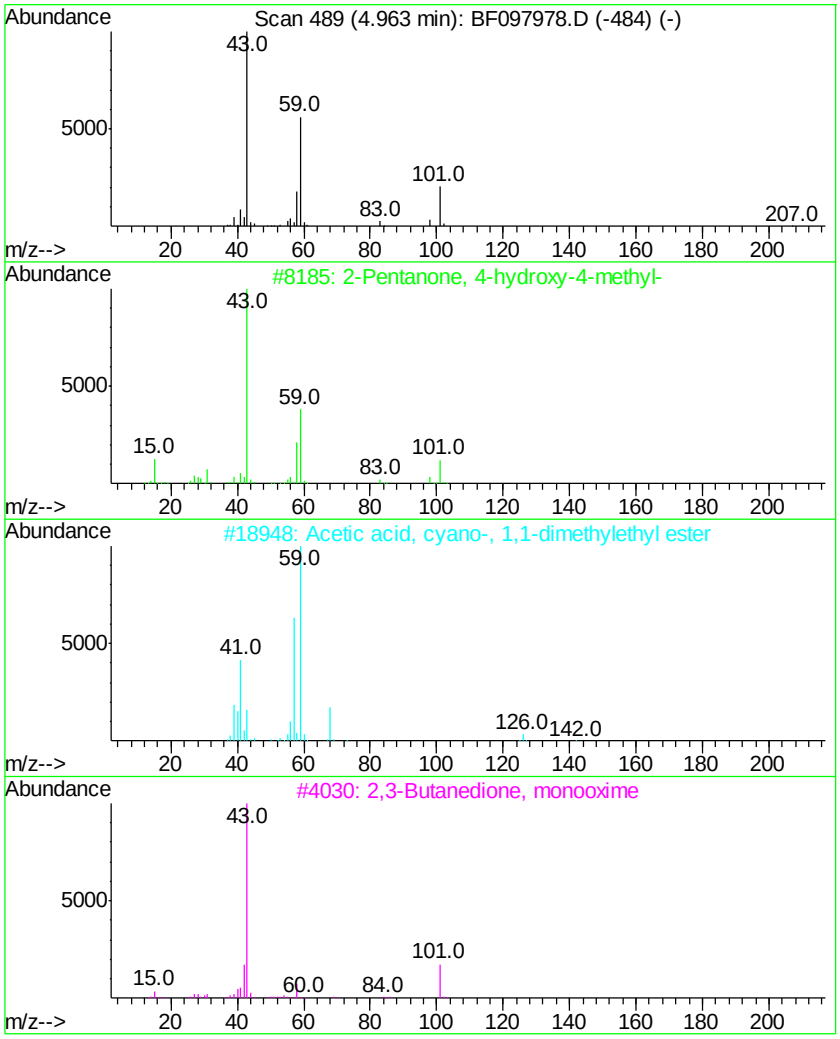
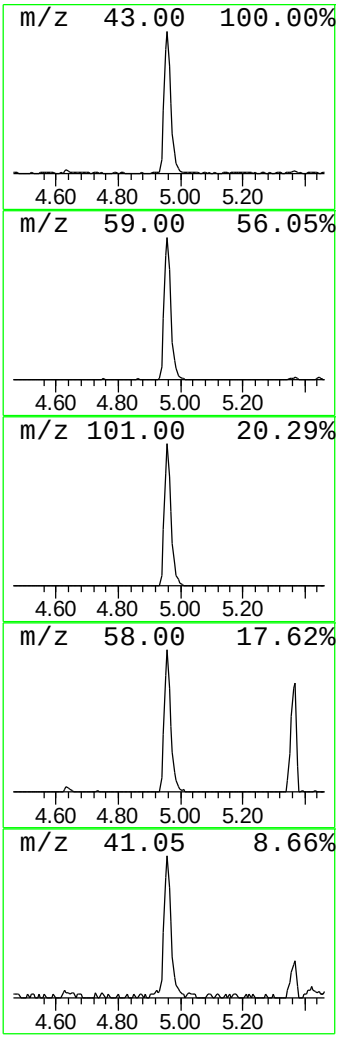
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	11.00 ng	477088	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : I4910-04
Misc :
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Instrument : BNA_F
ClientSampleId : SP-7-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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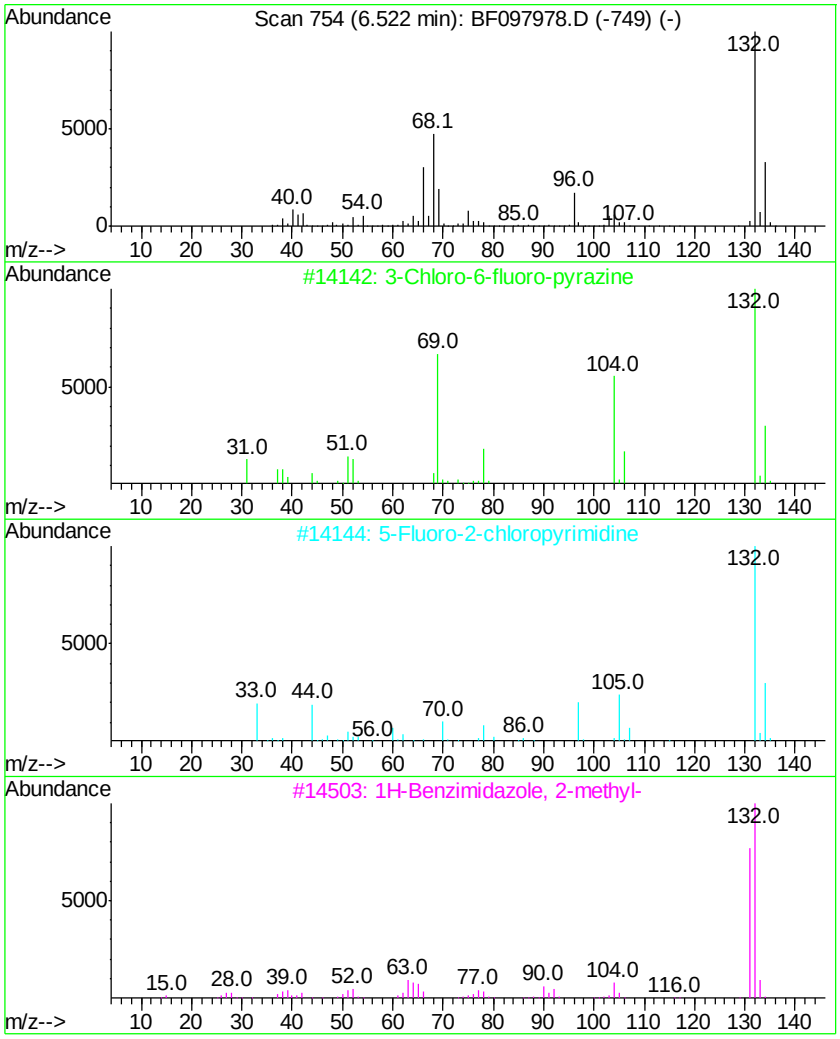
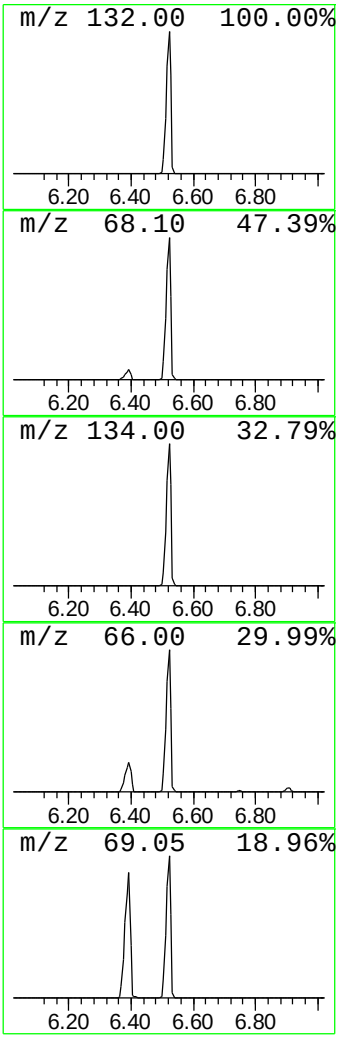
Peak Number 3 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	84.25 ng	3652820	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	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 : SP-7-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
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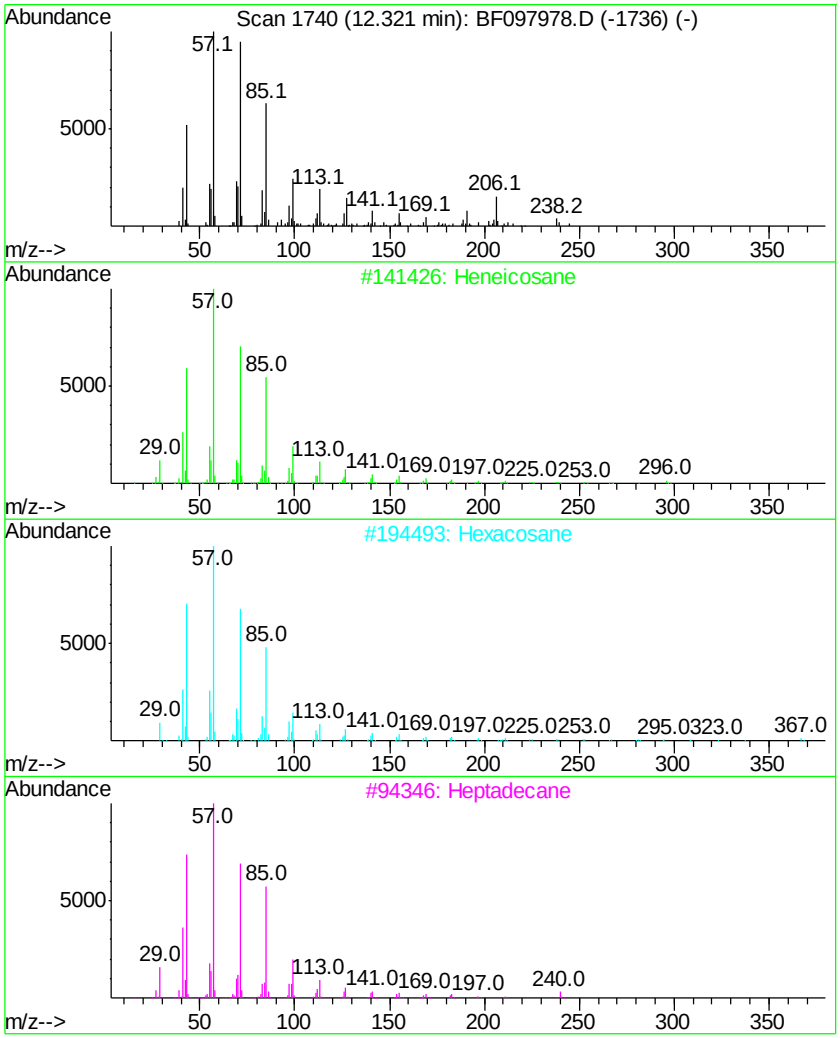
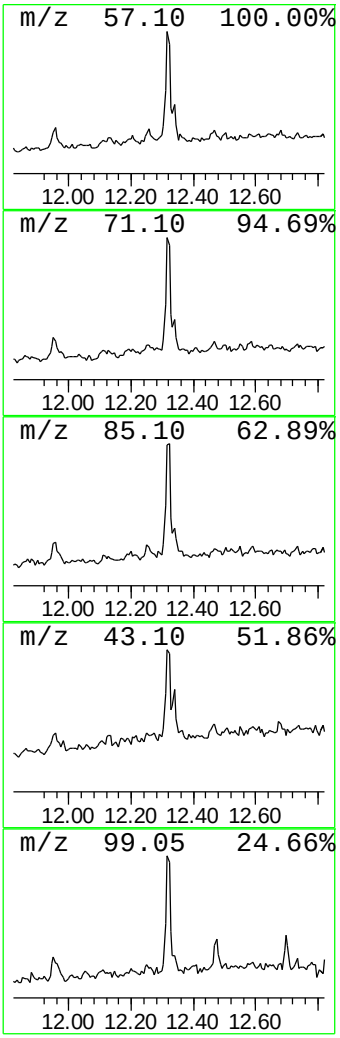
Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	4.00 ng	184222	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	74
2	Hexacosane	366	C26H54	000630-01-3	74
3	Heptadecane	240	C17H36	000629-78-7	72
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	72
5	Hexadecane	226	C16H34	000544-76-3	64





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
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Sample : I4910-04
Misc :
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Instrument : BNA_F
ClientSampleId : SP-7-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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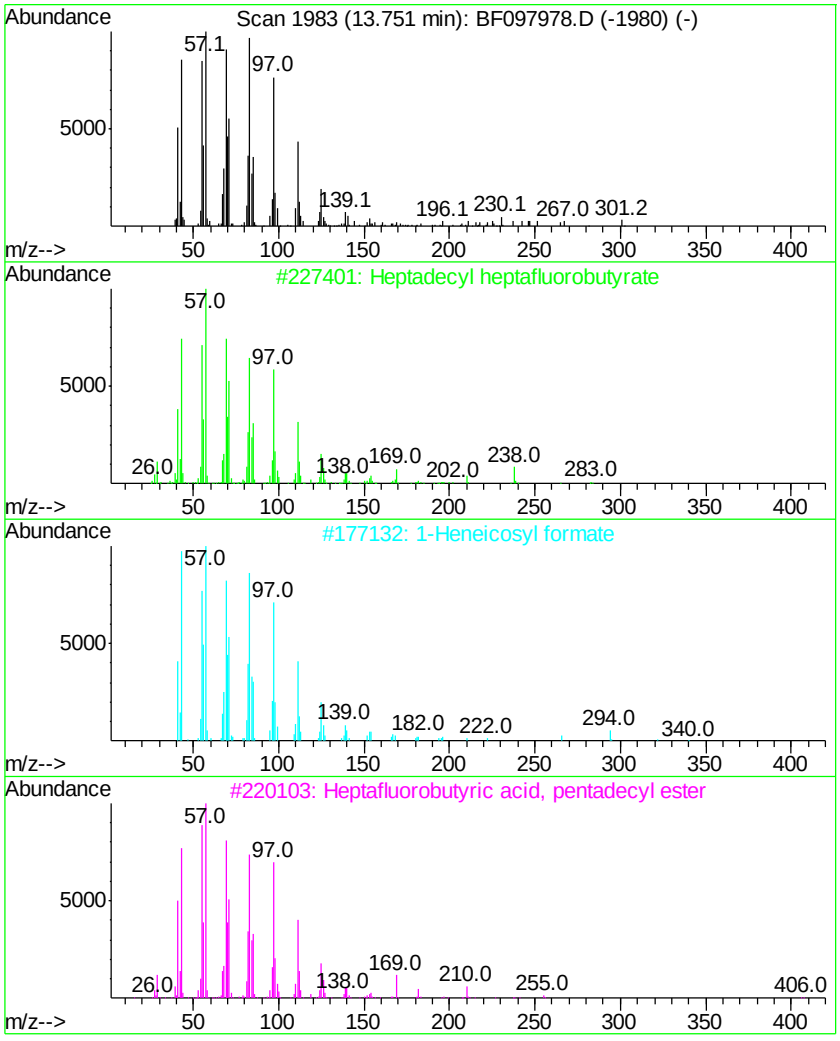
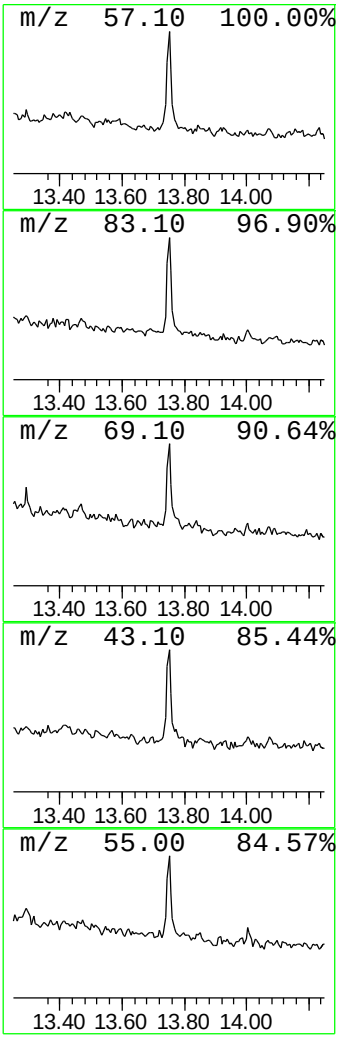
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	4.04 ng	175982	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	1-Nonadecene	266	C19H38	018435-45-5	91





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7-8

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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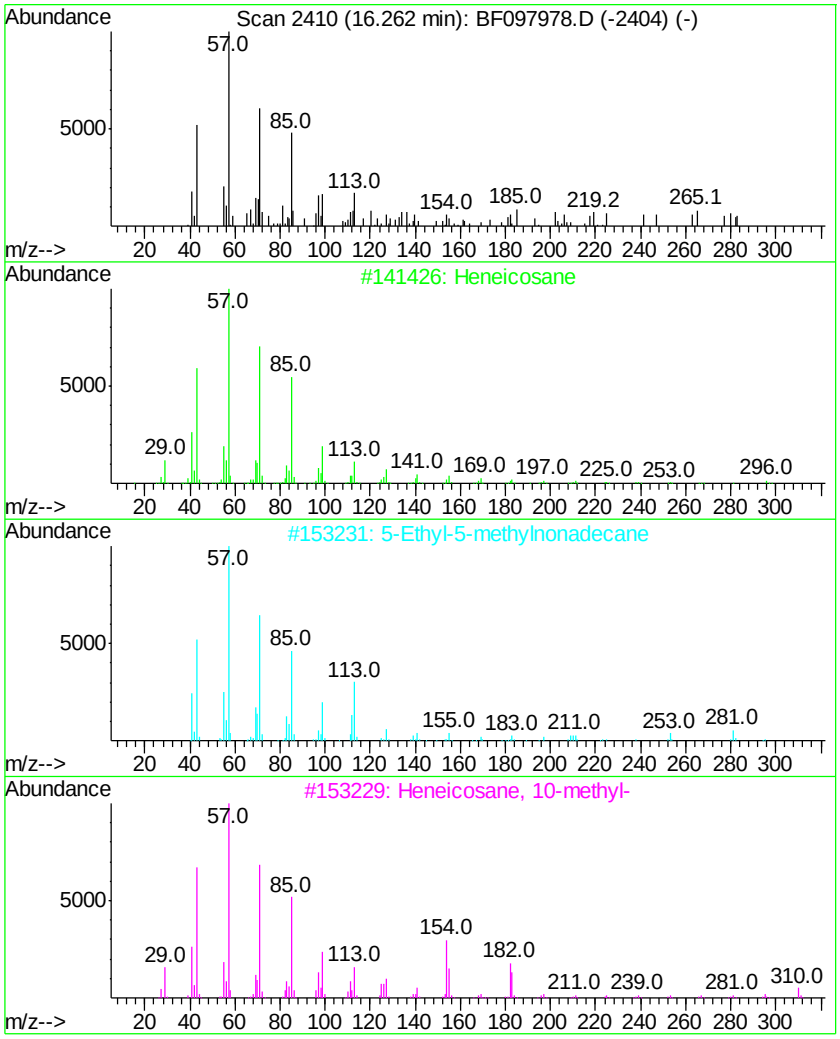
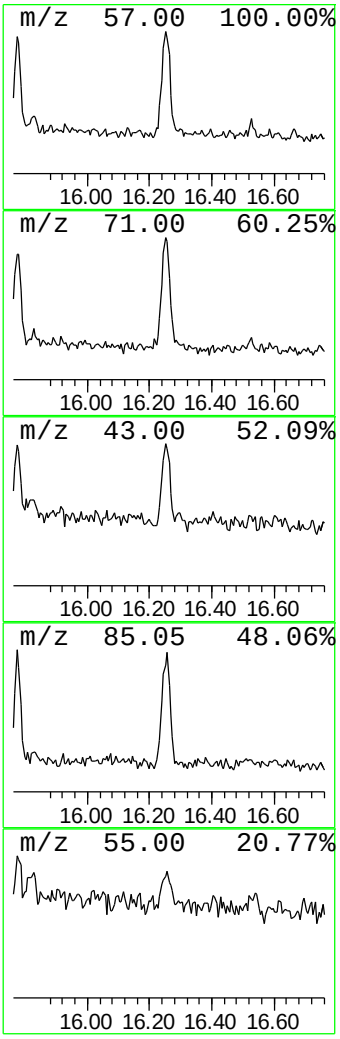
Peak Number 8 5-Ethyl-5-methylnonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.26	2.44 ng	79508	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	72
2	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	64
3	Heneicosane, 10-methyl-	310	C22H46	013287-25-7	64
4	Heptadecane	240	C17H36	000629-78-7	59
5	Hexacosane	366	C26H54	000630-01-3	58





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
unknown3.15	3.15	3.2	ng	137865	1	6.75	867107	20.0
2-Pentanone, 4-hy...	4.96	11.0	ng	477088	1	6.75	867107	20.0
unknown6.52	6.52	84.3	ng	3652820	1	6.75	867107	20.0
Heneicosane	12.32	4.0	ng	184222	4	11.26	920691	20.0
Heptadecyl heptaf...	13.75	4.0	ng	175982	5	13.90	871844	20.0
5-Ethyl-5-methyln...	16.26	2.4	ng	79508	6	15.32	652541	20.0