LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089987.D
Acq On : 2 Sep 2016 20:57
Operator : UM/SJ
Sample : H4675-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEMP-AB(0-2)-4

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-BF083116.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	1.632	3	4	13	rVV	441538	830494	16.37%	1.645%
2	1.747	13	14	33	rVV	2195080	4967339	97.94%	9.840%
3	1.998	33	36	42	rVB2	66072	191281	3.77%	0.379%
4	4.776	276	279	289	rBV	755021	1229486	24.24%	2.436%
5	5.221	314	318	320	rBV	4256808	4917185	96.95%	9.741%
6	6.284	407	411	413	rBV	4239929	5072019	100.00%	10.048%
7	6.399	418	421	424	rVV	3577769	4698953	92.64%	9.309%
8	6.639	440	442	444	rBV	1162808	1096910	21.63%	2.173%
9	6.799	453	456	458	rBV	2578930	3524416	69.49%	6.982%
10	7.199	488	491	494	rBV	2122664	3118690	61.49%	6.178%
11	7.324	498	502	510	rVV	94457	166254	3.28%	0.329%
12	7.919	552	554	557	rBV	1595694	1385487	27.32%	2.745%
13	9.005	646	649	651	rBV	4240482	5015668	98.89%	9.936%
14	9.393	681	683	686	rBV	1641186	1747190	34.45%	3.461%
15	9.622	701	703	704	rBV	72387	56472	1.11%	0.112%
16	9.668	704	707	709	rBV	1662444	1550901	30.58%	3.072%
17	10.113	745	746	748	rVB	104849	109954	2.17%	0.218%
18	10.342	763	766	769	rBV	40533	83342	1.64%	0.165%
19	10.445	772	775	778	rBV2	2303236	2627229	51.80%	5.205%
20	10.582	786	787	792	rBV	97593	187411	3.69%	0.371%
21	10.776	802	804	809	rBV2	21777	50893	1.00%	0.101%
22	11.028	824	826	828	rBV	53098	71210	1.40%	0.141%
23	11.131	833	835	838	rBV2	1129786	1358962	26.79%	2.692%
24	11.393	855	858	861	rBV	45697	78435	1.55%	0.155%
25	11.691	882	884	885	rBV	54028	52187	1.03%	0.103%
26	12.719	971	974	976	rBV	3599839	3374290	66.53%	6.684%
27	13.634	1051	1054	1058	rVB	207763	277029	5.46%	0.549%
28	13.748	1062	1064	1067	rBV	1262311	1215931	23.97%	2.409%
29	14.262	1105	1109	1113	rBV4	28066	89018	1.76%	0.176%
30	15.097	1180	1182	1185	rBV	969679	1106815	21.82%	2.193%
31	15.531	1218	1220	1222	rBV	36213	54752	1.08%	0.108%
32	15.577	1222	1224	1228	rVB4	30141	65280	1.29%	0.129%
33	17.508	1389	1393	1397	rBV7	34158	108082	2.13%	0.214%

LSC Area Percent Report

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Instrument :
BNA_F
ClientSampleId :
TEMP-AB(0-2)-4

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-BF083116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

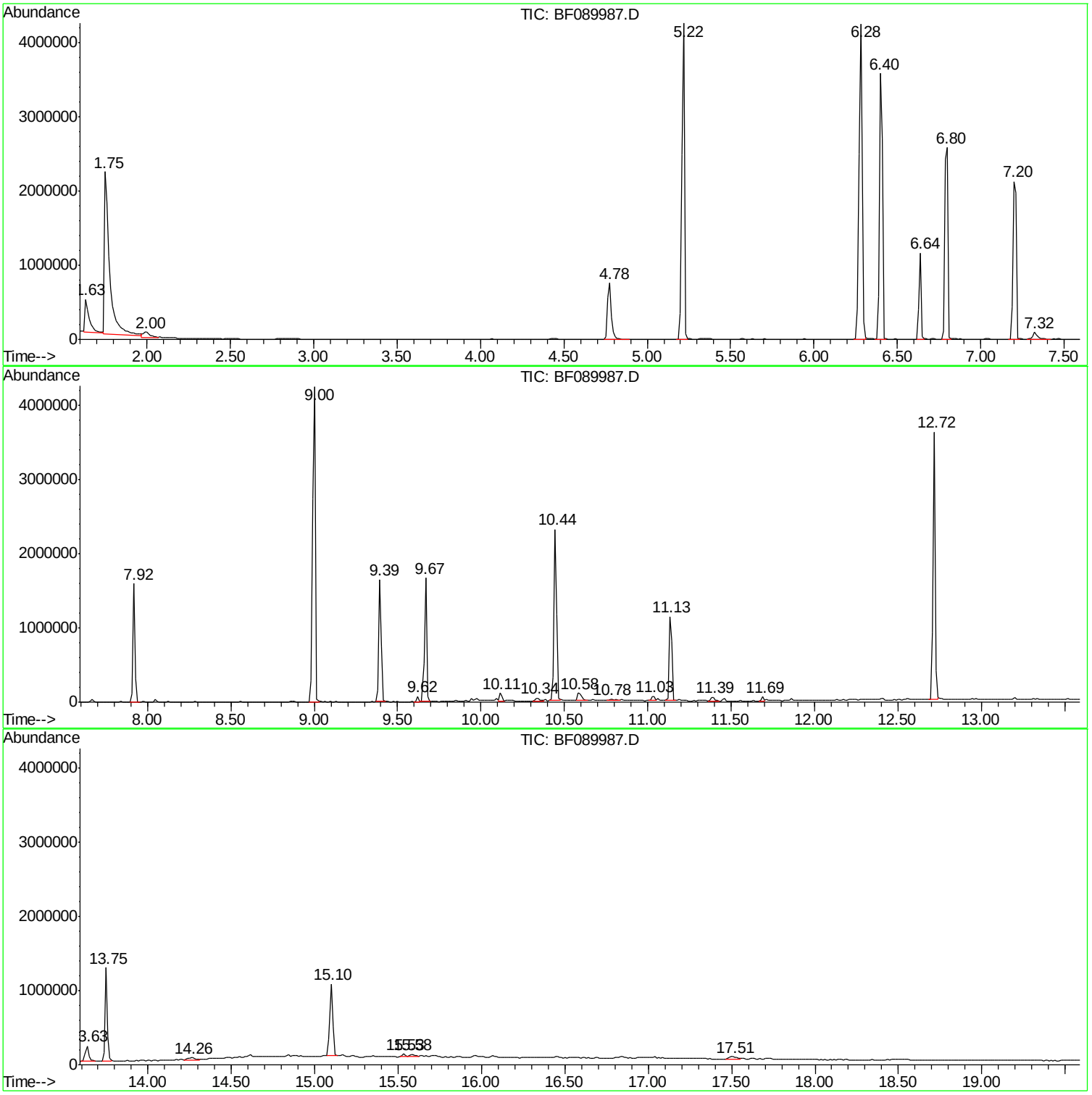
Sum of corrected areas: 50479565

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089987.D
Acq On : 2 Sep 2016 20:57
Operator : UM/SJ
Sample : H4675-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEMP-AB(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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

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Operator : UM/SJ
Sample : H4675-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEMP-AB(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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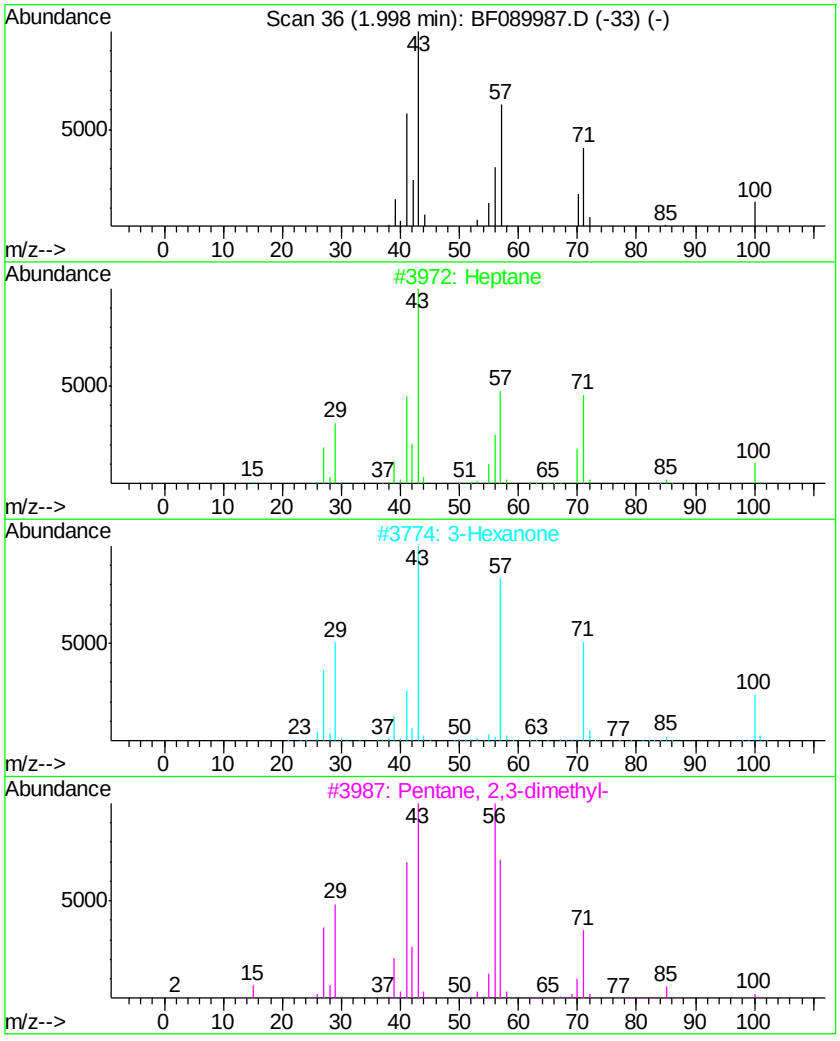
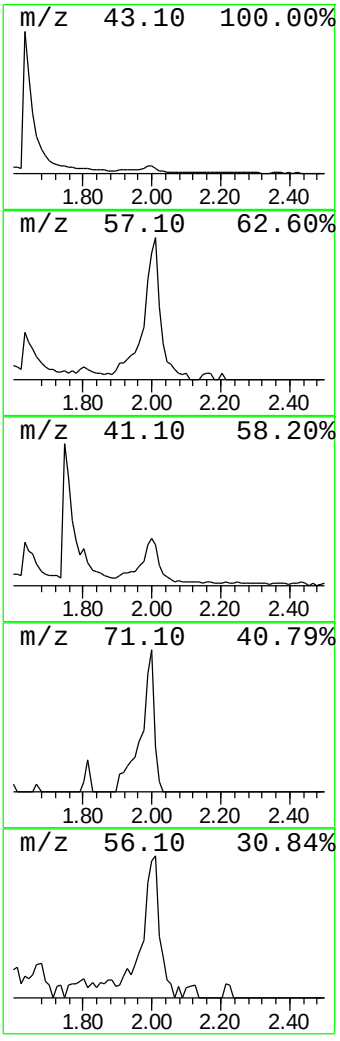
Peak Number 3 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	3.49 ng	191281	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	3-Hexanone	100	C6H12O	000589-38-8	47
3	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	45
4	Octane	114	C8H18	000111-65-9	42
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090216\
Data File : BF089987.D
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Operator : UM/SJ
Sample : H4675-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEMP-AB(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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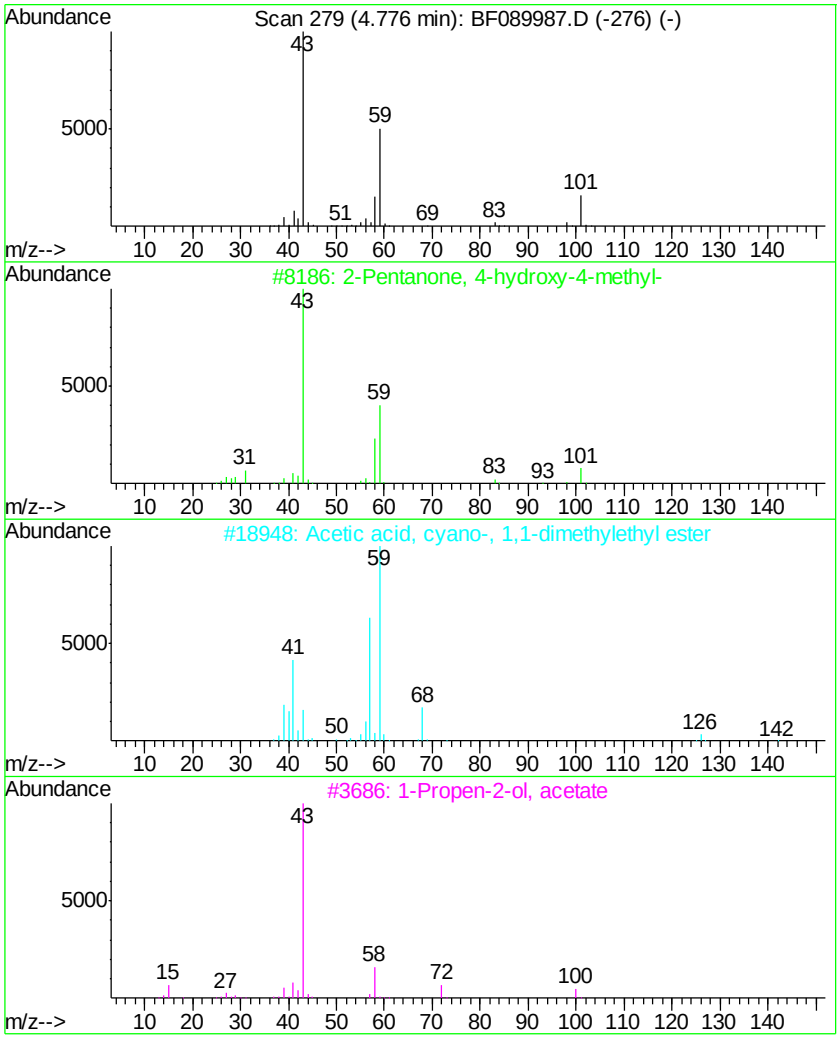
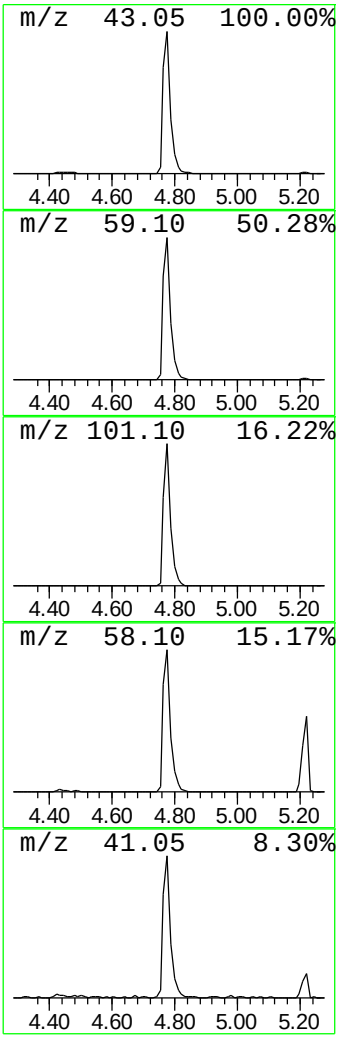
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	22.42 ng	1229490	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TEMP-AB(0-2)-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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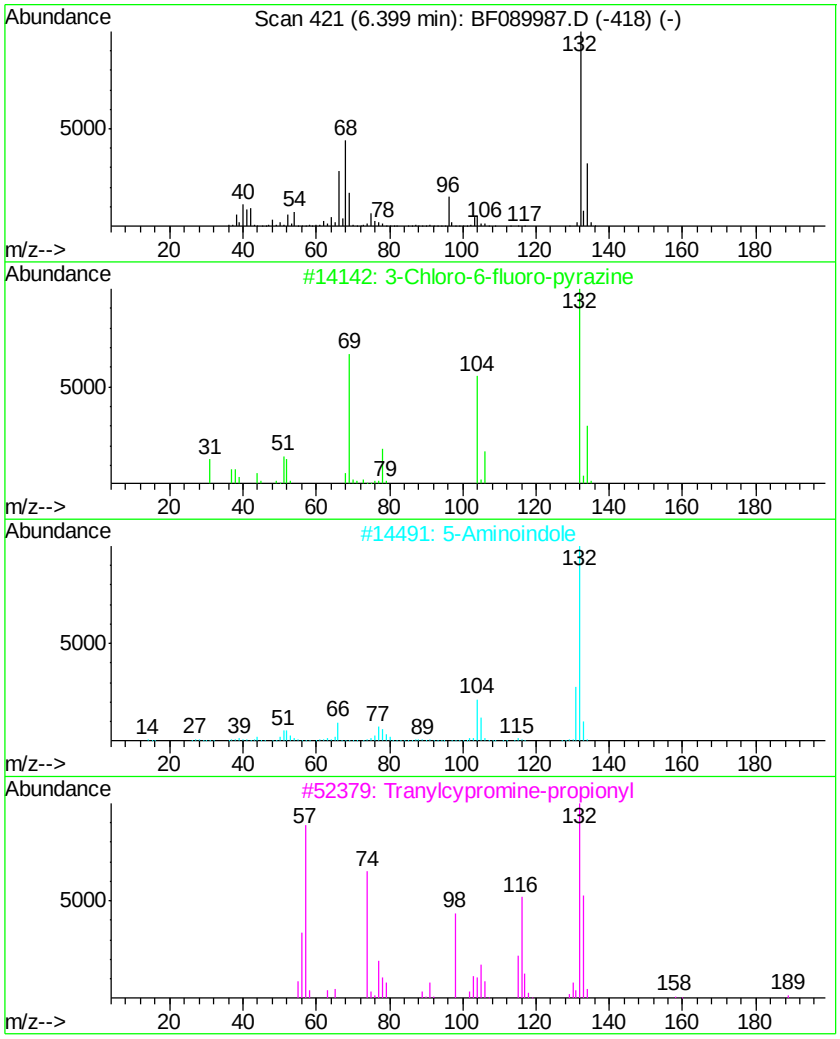
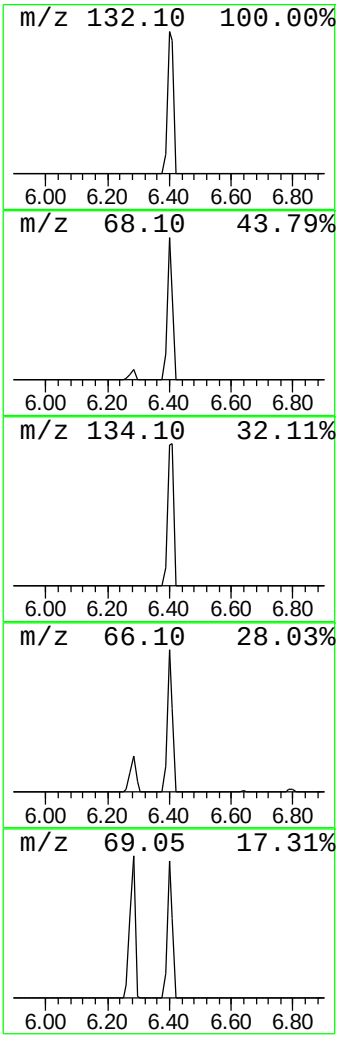
Peak Number 5 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	85.68 ng	4698950	1,4-Dichlorobenzene-d4	6.64

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
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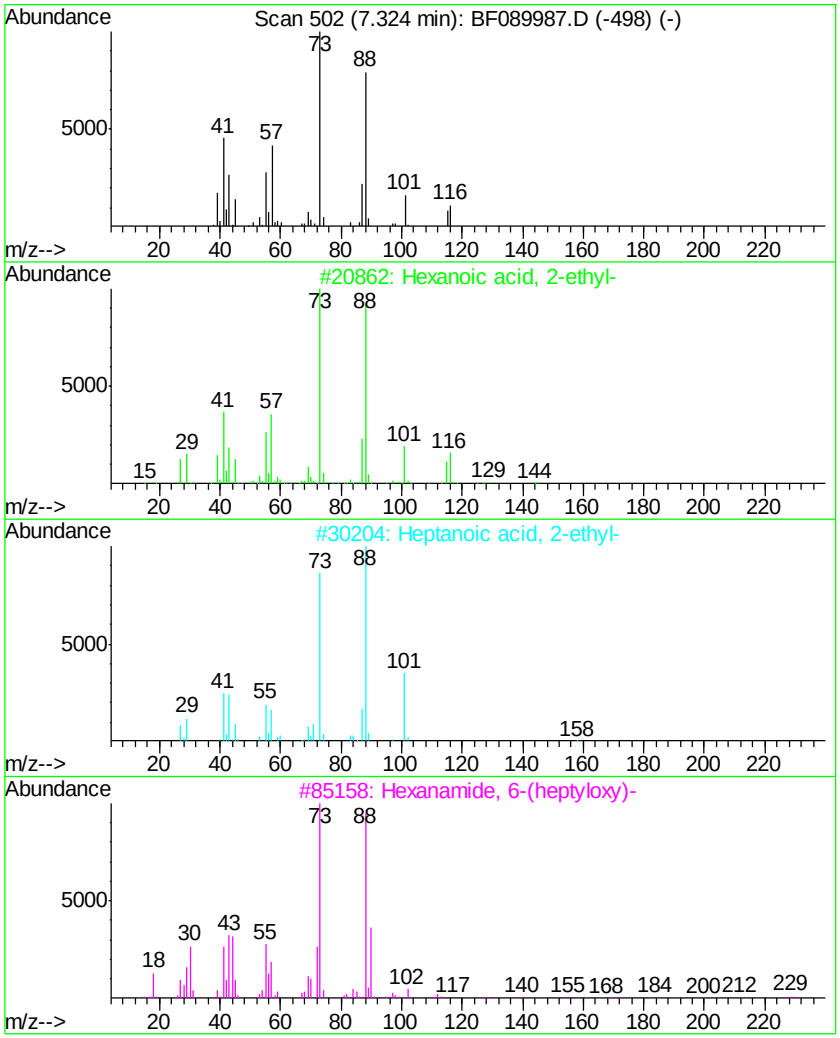
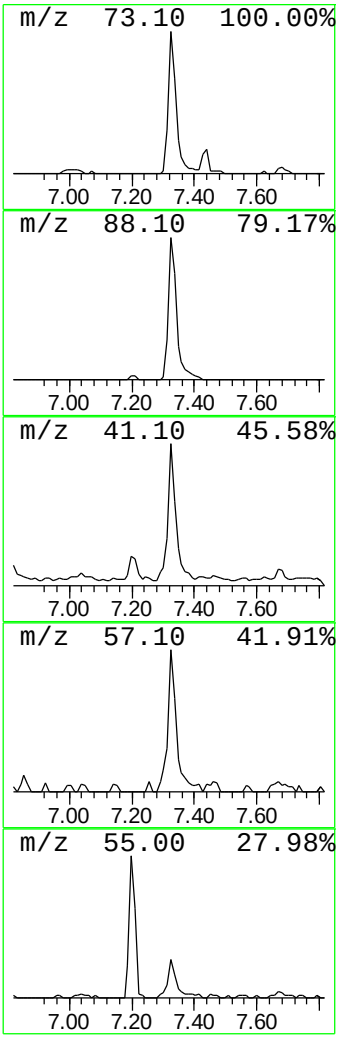
Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	2.40 ng	166254	Naphthalene-d8	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	40
4	1,4-Dioxane	88	C4H8O2	000123-91-1	40
5	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	36





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TIC Library : C:\Database\NIST11.L
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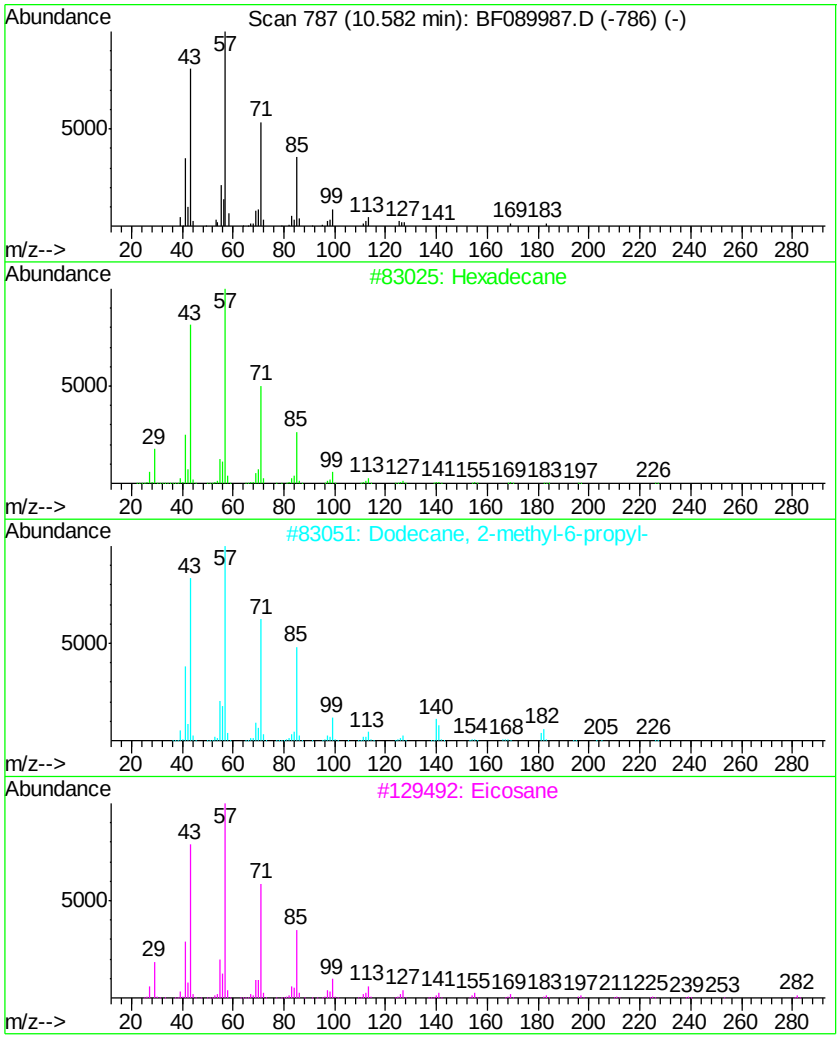
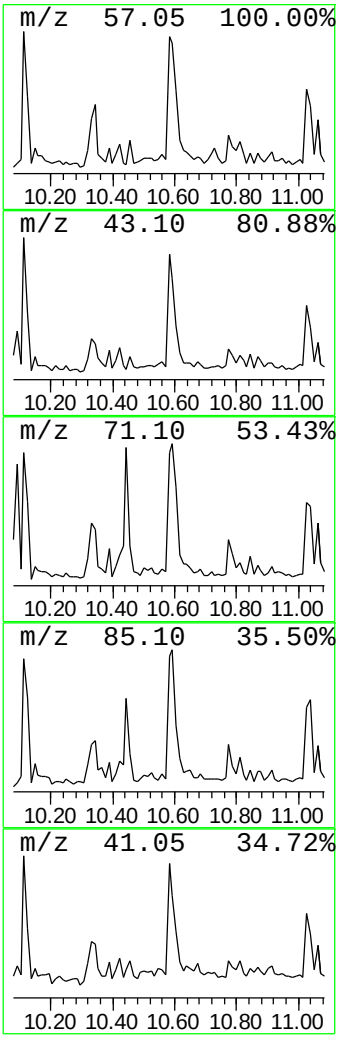
****

Peak Number 8 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	2.76 ng	187411	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3	Eicosane	282	C20H42	000112-95-8	80
4	Heptadecane	240	C17H36	000629-78-7	78
5	Pentadecane	212	C15H32	000629-62-9	72





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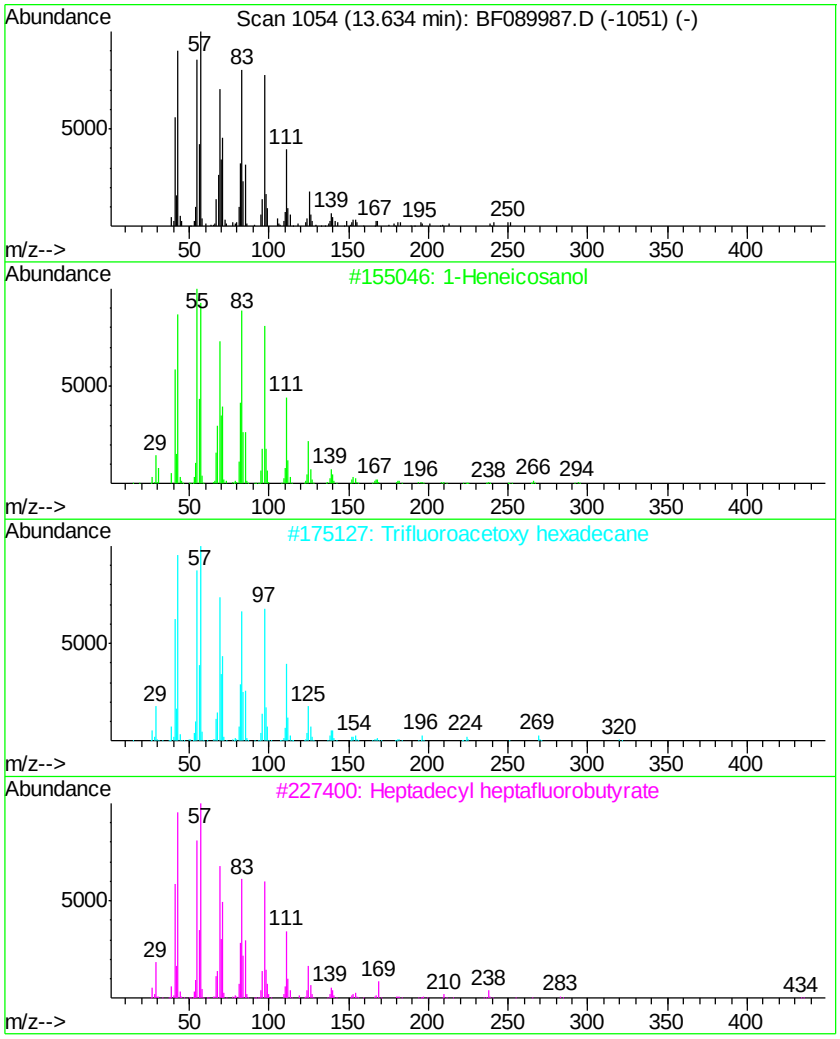
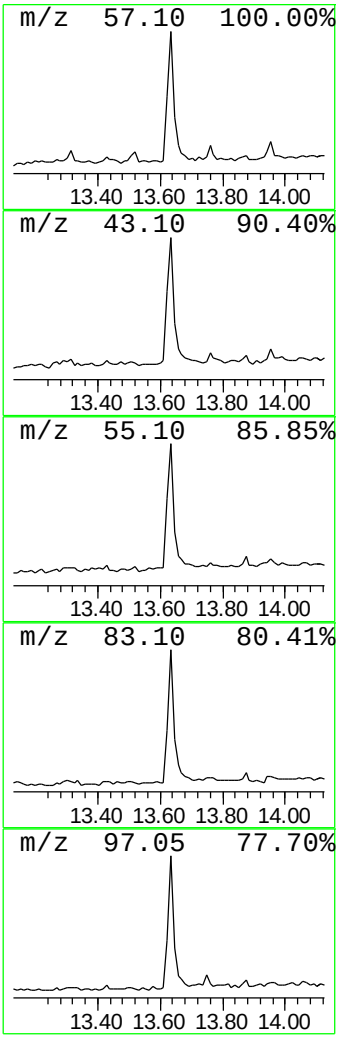
Peak Number 9 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	4.56 ng	277029	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	93





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
Heptane	2.00	3.5	ng	191281	1	6.64	1096910	20.0
2-Pentanone, 4-hy...	4.78	22.4	ng	1229490	1	6.64	1096910	20.0
unknown6.40	6.40	85.7	ng	4698950	1	6.64	1096910	20.0
Hexanoic acid, 2-...	7.32	2.4	ng	166254	2	7.92	1385490	20.0
Hexadecane	10.58	2.8	ng	187411	4	11.13	1358960	20.0
1-Heneicosanol	13.63	4.6	ng	277029	5	13.75	1215930	20.0