LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096796.D
Acq On : 15 Jul 2017 2:43
Operator : SJ/JU
Sample : I4187-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB6-0-2

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-BF071317.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	2.922	157	159	167	rBV	14474	31242	1.26%	0.151%
2	4.134	360	365	373	rBV2	17638	28359	1.14%	0.137%
3	4.804	474	479	490	rVB	342999	481951	19.43%	2.336%
4	5.240	548	553	556	rBV	2403866	2479900	100.00%	12.020%
5	6.275	720	729	732	rBV	2189782	2239649	90.31%	10.855%
6	6.398	745	750	753	rBV	2394393	2212505	89.22%	10.724%
7	6.622	785	788	792	rBV	740591	611877	24.67%	2.966%
8	6.781	811	815	818	rBV	1926917	1699001	68.51%	8.235%
9	7.187	879	884	887	rBV	1470790	1382154	55.73%	6.699%
10	7.304	898	904	910	rBV	38504	41776	1.68%	0.202%
11	7.904	1002	1006	1010	rBV	1001393	815333	32.88%	3.952%
12	8.986	1185	1190	1193	rBV	2550488	2320628	93.58%	11.248%
13	9.375	1253	1256	1260	rBV	419759	338505	13.65%	1.641%
14	9.657	1299	1304	1307	rBV	889148	833997	33.63%	4.042%
15	10.439	1433	1437	1440	rBV	1243245	1077825	43.46%	5.224%
16	10.575	1457	1460	1467	rBV	49940	51517	2.08%	0.250%
17	11.022	1532	1536	1539	rBV	39280	32765	1.32%	0.159%
18	11.128	1551	1554	1557	rBV	683150	590906	23.83%	2.864%
19	11.675	1642	1647	1650	rBV3	33266	31918	1.29%	0.155%
20	12.333	1757	1759	1763	rVB	42036	36837	1.49%	0.179%
21	12.563	1793	1798	1801	rBV	42858	44459	1.79%	0.215%
22	12.716	1820	1824	1827	rBV	1514044	1384262	55.82%	6.709%
23	13.621	1972	1978	1984	rBV2	96983	143005	5.77%	0.693%
24	13.757	1997	2001	2004	rBV2	798241	749448	30.22%	3.632%
25	14.257	2082	2086	2090	rBV4	42192	53655	2.16%	0.260%
26	14.610	2143	2146	2149	rVB2	33034	31146	1.26%	0.151%
27	14.674	2154	2157	2160	rVB3	31304	29936	1.21%	0.145%
28	14.757	2168	2171	2178	rVB2	30155	53711	2.17%	0.260%
29	14.874	2188	2191	2197	rVB2	50068	62622	2.53%	0.304%
30	15.139	2231	2236	2240	rBV	504884	575765	23.22%	2.791%
31	15.580	2307	2311	2315	rVB	48365	58356	2.35%	0.283%
32	15.621	2315	2318	2324	rVB6	28065	48777	1.97%	0.236%
33	16.433	2450	2456	2459	rBV8	25628	58343	2.35%	0.283%

LSC Area Percent Report

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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CI-SB6-0-2

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-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 20632130

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
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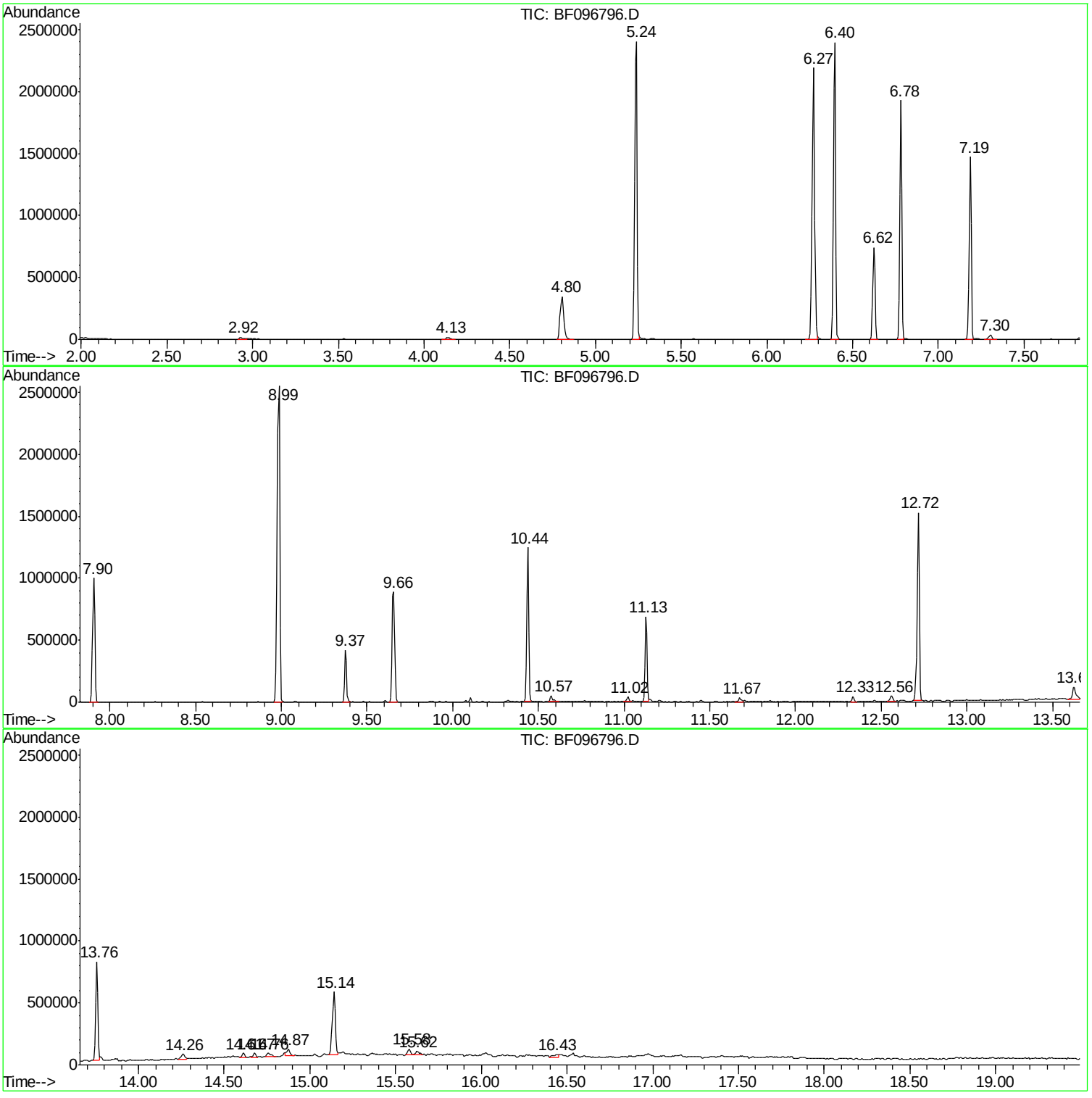
Acq On : 15 Jul 2017 2:43
Operator : SJ/JU
Sample : I4187-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CI-SB6-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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\BF071417\
Data File : BF096796.D
Acq On : 15 Jul 2017 2:43
Operator : SJ/JU
Sample : I4187-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB6-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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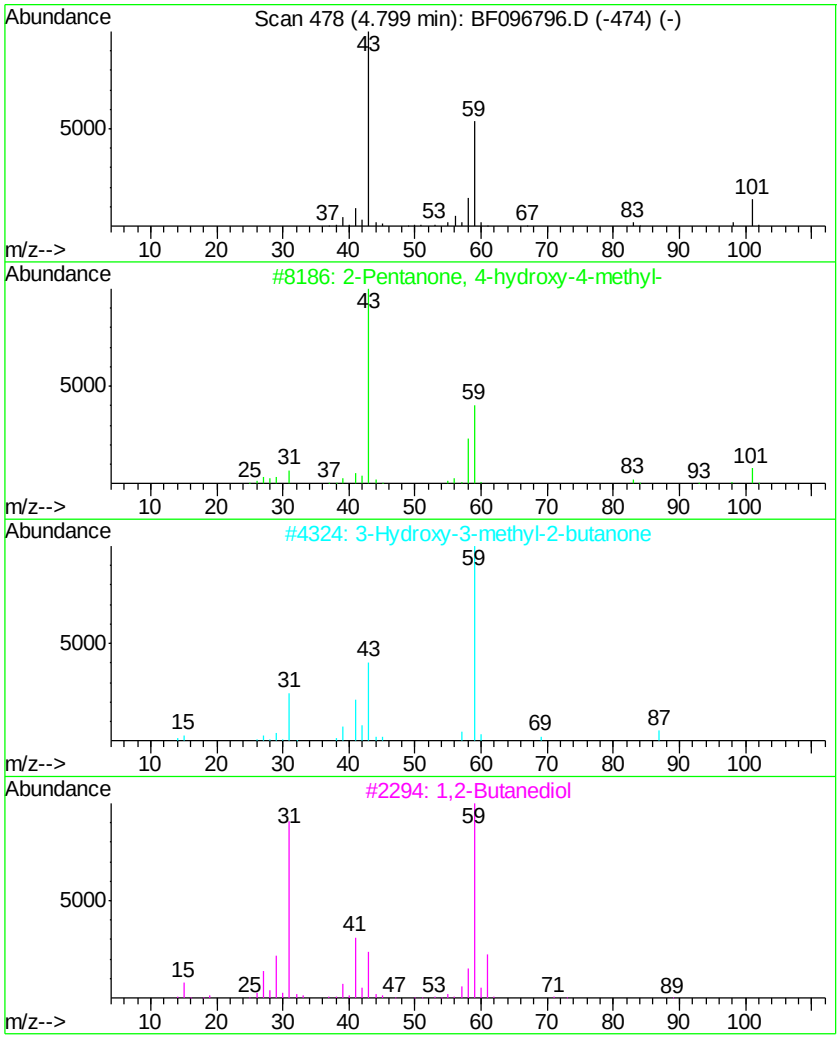
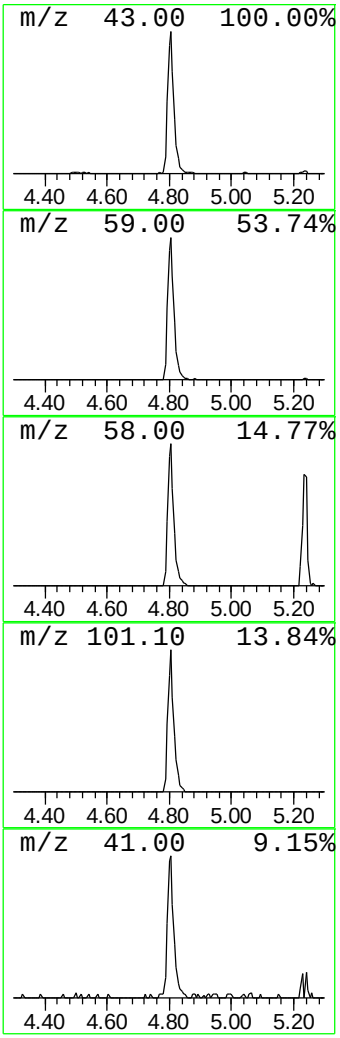
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	15.75 ng	481951	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
3	1,2-Butanediol	90	C4H10O2	000584-03-2	9
4	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096796.D
Acq On : 15 Jul 2017 2:43
Operator : SJ/JU
Sample : I4187-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB6-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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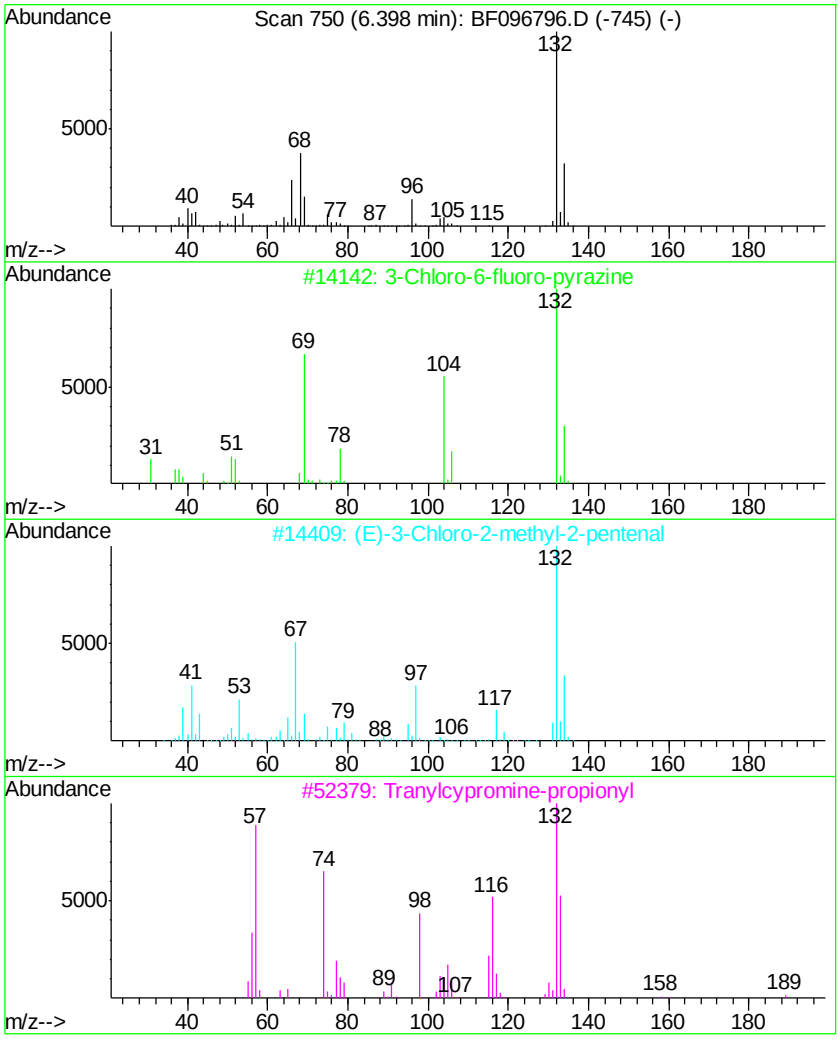
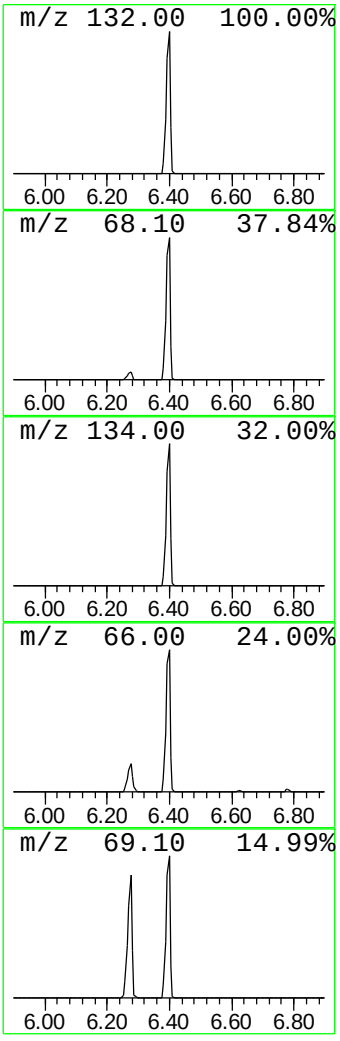
Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	72.32 ng	2212510	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Amphetaminil	250	C17H18N2	017590-01-1	12





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Sample : I4187-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CI-SB6-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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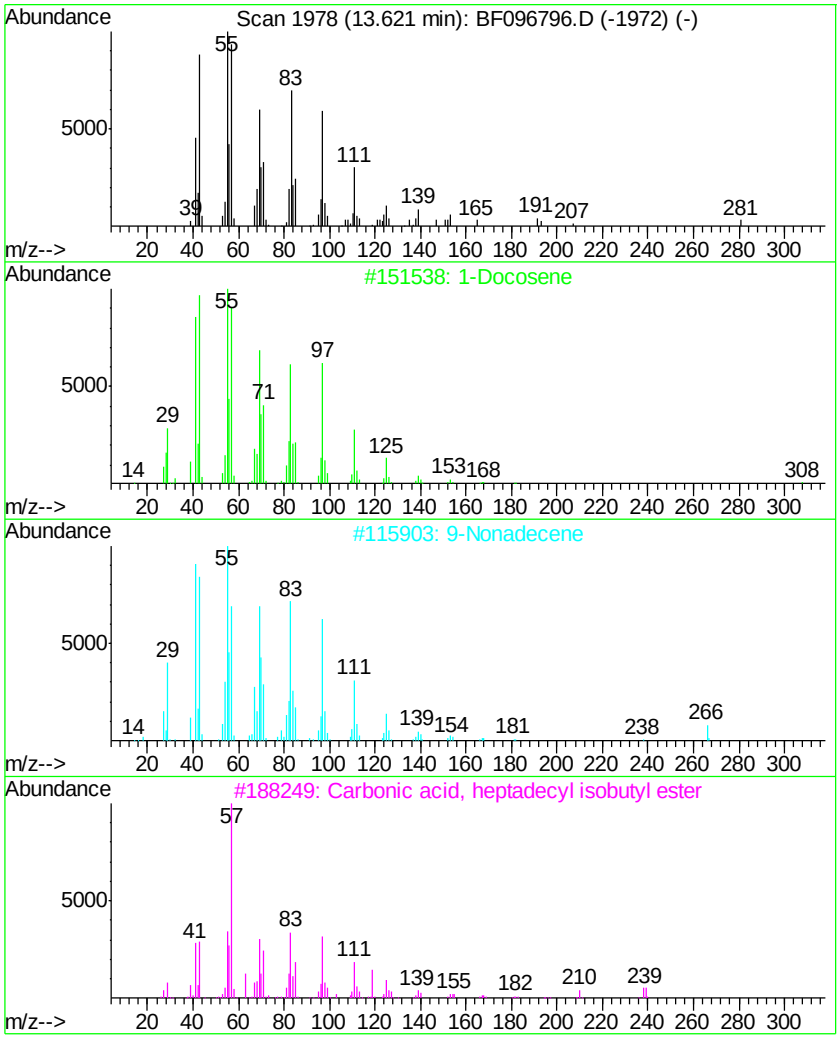
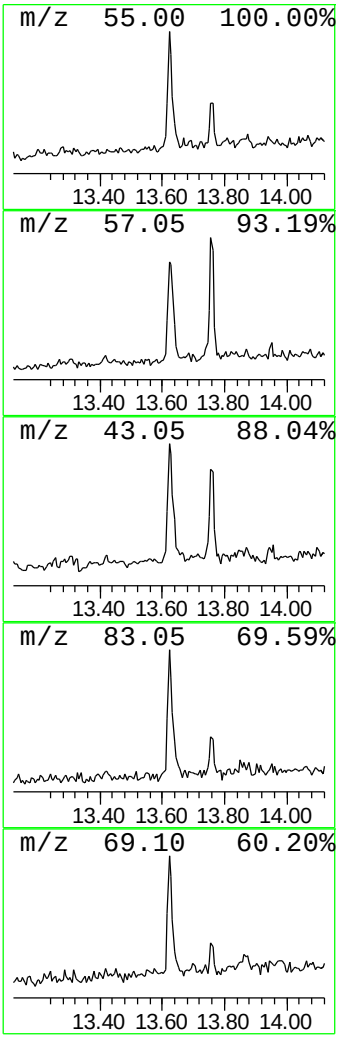
Peak Number 4 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	3.82 ng	143005	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	9-Nonadecene	266	C19H38	031035-07-1	91
3	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	90
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	86
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	74





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Sample : I4187-06
Misc :
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Instrument : BNA_F
ClientSampleId : CI-SB6-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
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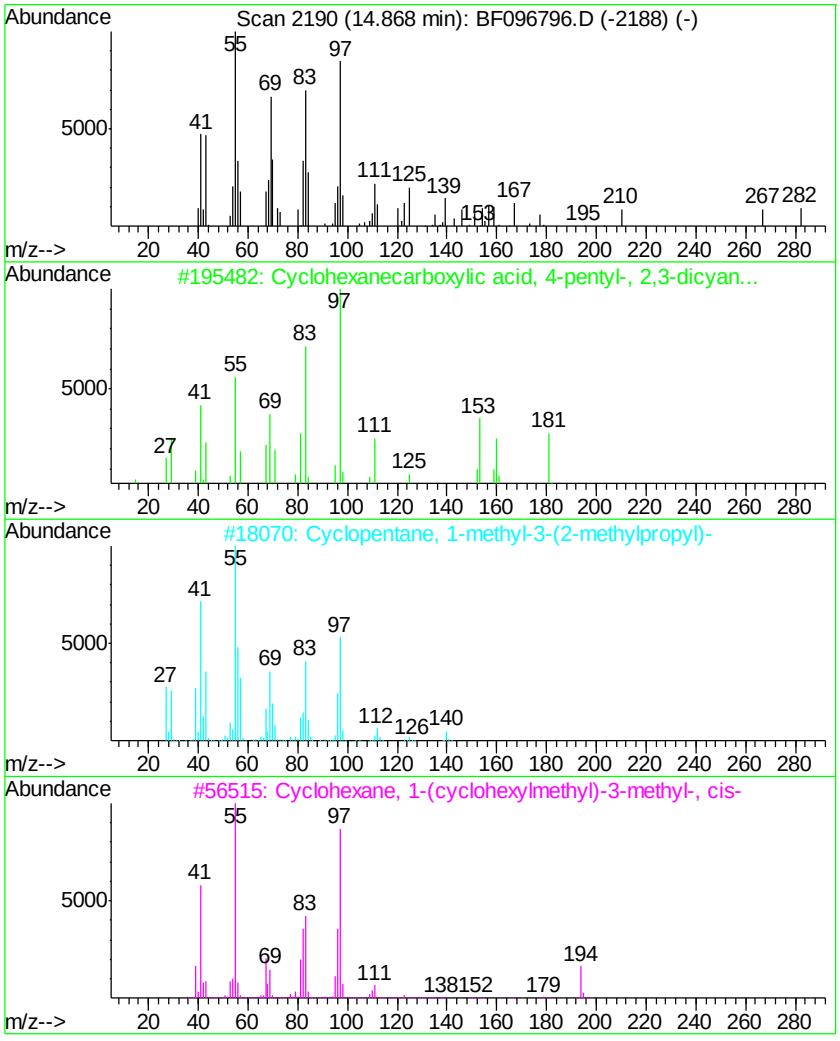
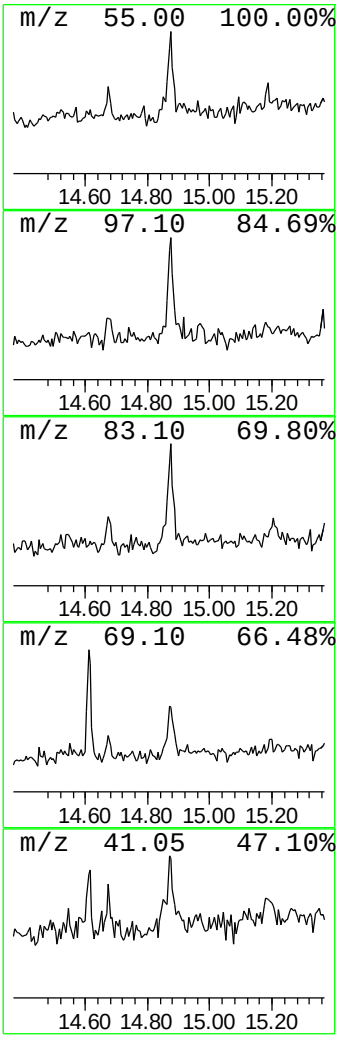
Peak Number 5 Cyclohexanecarboxylic acid,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.18 ng	62622	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 4-pe...	368	C22H28N2O3	133856-87-8	53
2	Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	46
3	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-96-0	43
4	Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	38
5	Cycloheptane, methyl-	112	C8H16	004126-78-7	35





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Sample : I4187-06
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CI-SB6-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

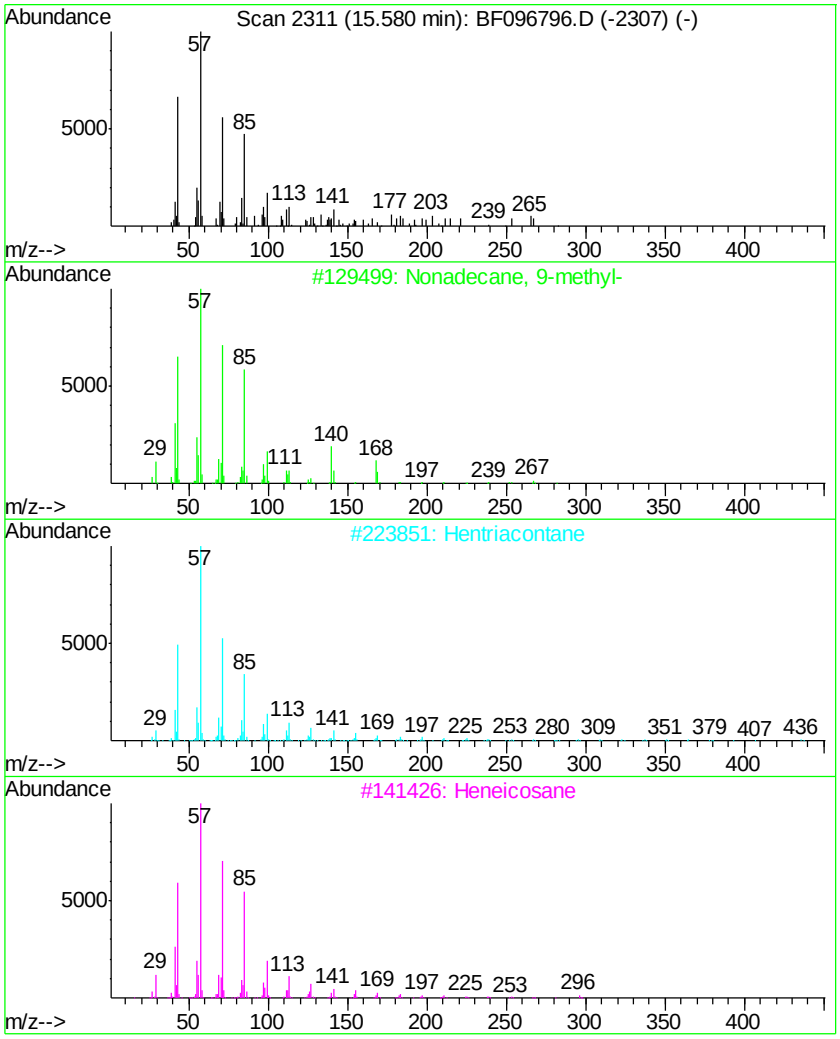
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

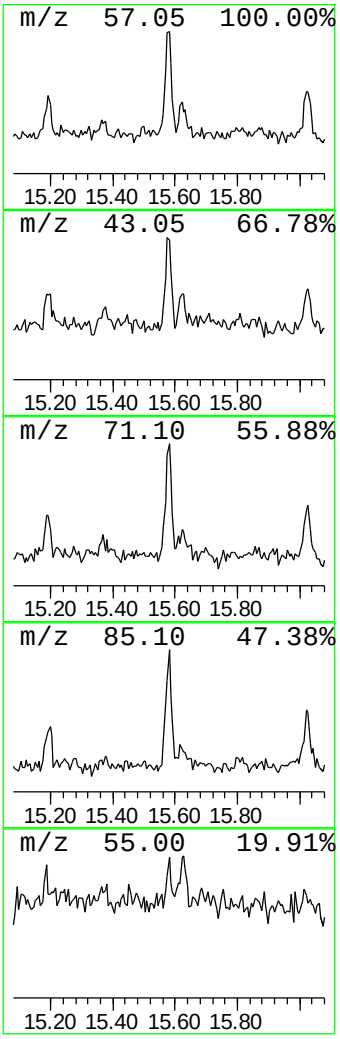
****

Peak Number 6 Nonadecane, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.03 ng	58356	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Hentriacontane	437	C31H64	000630-04-6	80
3	Heneicosane	296	C21H44	000629-94-7	72
4	Pentadecane	212	C15H32	000629-62-9	72
5	Octadecane	254	C18H38	000593-45-3	64





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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...	4.80	15.8	ng	481951	1	6.62	611877	20.0
unknown6.40	6.40	72.3	ng	2212510	1	6.62	611877	20.0
1-Docosene	13.62	3.8	ng	143005	5	13.76	749448	20.0
Cyclohexanecarbox...	14.87	2.2	ng	62622	6	15.14	575765	20.0
Nonadecane, 9-met...	15.58	2.0	ng	58356	6	15.14	575765	20.0