LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092891.D
Acq On : 10 Feb 2017 19:01
Operator : SJ/MA
Sample : I1777-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-11-13

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-BF013017.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	5.070	258	261	270	rBV	1048586	1432368	33.99%	3.815%
2	5.493	295	298	301	rBV	2848509	3301783	78.35%	8.793%
3	6.533	386	389	392	rBV	3256767	3685576	87.46%	9.815%
4	6.602	393	395	398	rVB	127157	124093	2.94%	0.330%
5	6.659	398	400	403	rBV	2876455	3435337	81.52%	9.149%
6	6.887	418	420	423	rBV	804225	972608	23.08%	2.590%
7	7.047	432	434	437	rBV	2760856	2619000	62.15%	6.975%
8	7.459	467	470	472	rBV	2203350	2169631	51.48%	5.778%
9	8.179	530	533	536	rBV	1480175	1328122	31.52%	3.537%
10	9.253	624	627	630	rBV	2834197	4214212	100.00%	11.223%
11	9.653	659	662	664	rBV	501547	448504	10.64%	1.194%
12	9.859	672	680	684	rBV	152965	325714	7.73%	0.867%
13	9.939	684	687	689	rVB	1614836	1710304	40.58%	4.555%
14	10.339	716	722	723	rBV2	51232	84213	2.00%	0.224%
15	10.362	723	724	726	rVB	126791	107458	2.55%	0.286%
16	10.579	741	743	747	rBV	37542	64767	1.54%	0.172%
17	10.728	753	756	758	rBV	2163714	2338355	55.49%	6.227%
18	10.842	764	766	770	rVB	108315	192207	4.56%	0.512%
19	11.288	803	805	806	rBV	124676	129903	3.08%	0.346%
20	11.425	814	817	819	rBV	1318564	1583405	37.57%	4.217%
21	11.711	840	842	844	rBV	136488	114128	2.71%	0.304%
22	12.111	875	877	880	rVB	35771	50700	1.20%	0.135%
23	12.465	906	908	910	rBV	91568	98092	2.33%	0.261%
24	13.014	953	956	958	rBV	2804608	3907061	92.71%	10.405%
25	13.482	991	997	1002	rBV	66720	145033	3.44%	0.386%
26	13.894	1031	1033	1041	rBV	105992	179548	4.26%	0.478%
27	14.054	1045	1047	1050	rVB	1330654	1315812	31.22%	3.504%
28	14.522	1083	1088	1089	rBV2	49035	121331	2.88%	0.323%
29	14.808	1111	1113	1117	rBV2	88841	141090	3.35%	0.376%
30	14.900	1119	1121	1123	rVV	62838	73471	1.74%	0.196%
31	15.505	1171	1174	1178	rBV	820609	1088154	25.82%	2.898%
32	16.431	1252	1255	1266	rVB4	18276	46900	1.11%	0.125%

LSC Area Percent Report

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Data File : BF092891.D
Acq On : 10 Feb 2017 19:01
Operator : SJ/MA
Sample : I1777-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38-SB-03-11-13

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-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

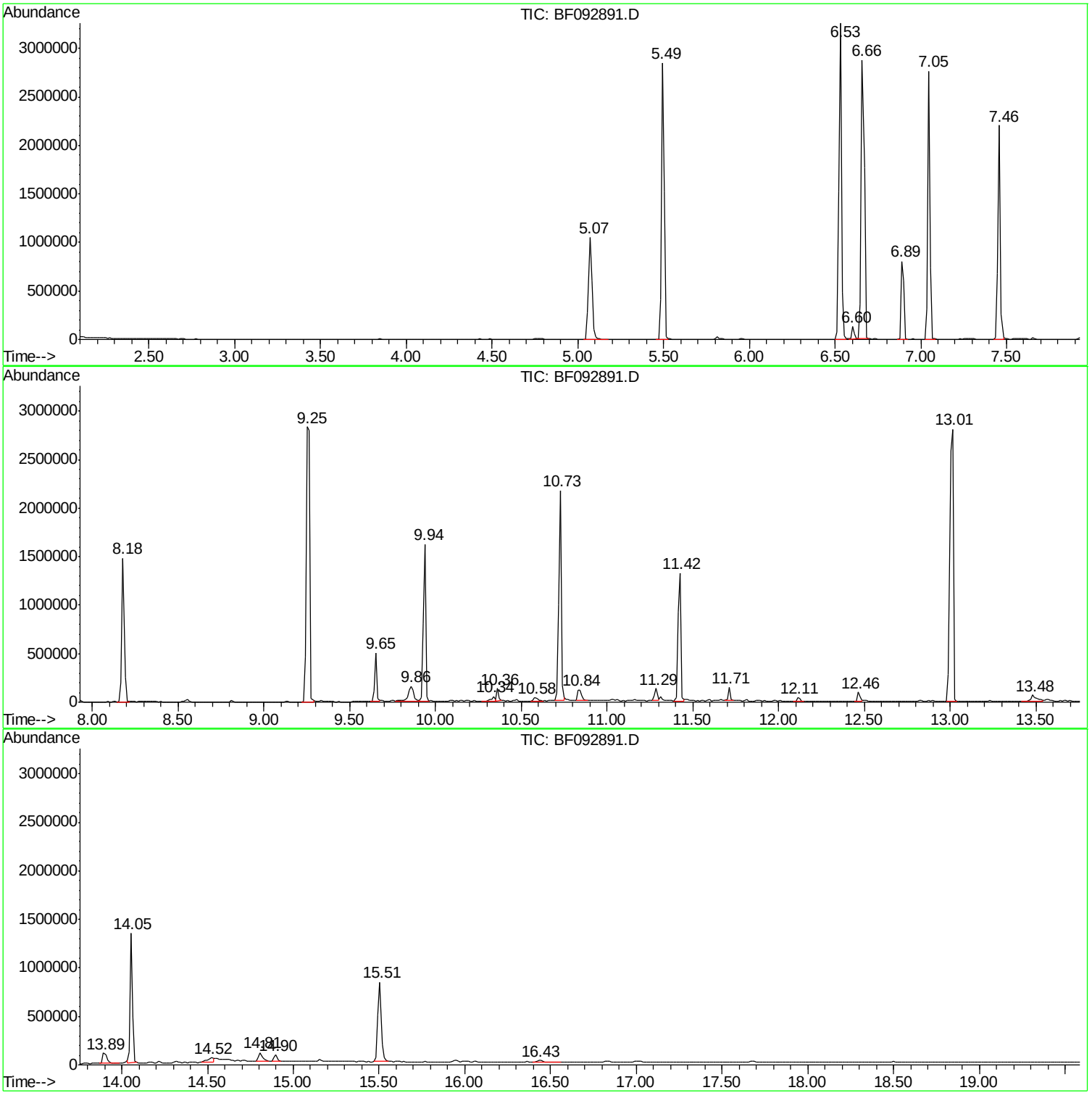
Sum of corrected areas: 37548880

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092891.D
Acq On : 10 Feb 2017 19:01
Operator : SJ/MA
Sample : I1777-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-11-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092891.D
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Sample : I1777-06
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Instrument : BNA_F
ClientSampleId : 38-SB-03-11-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

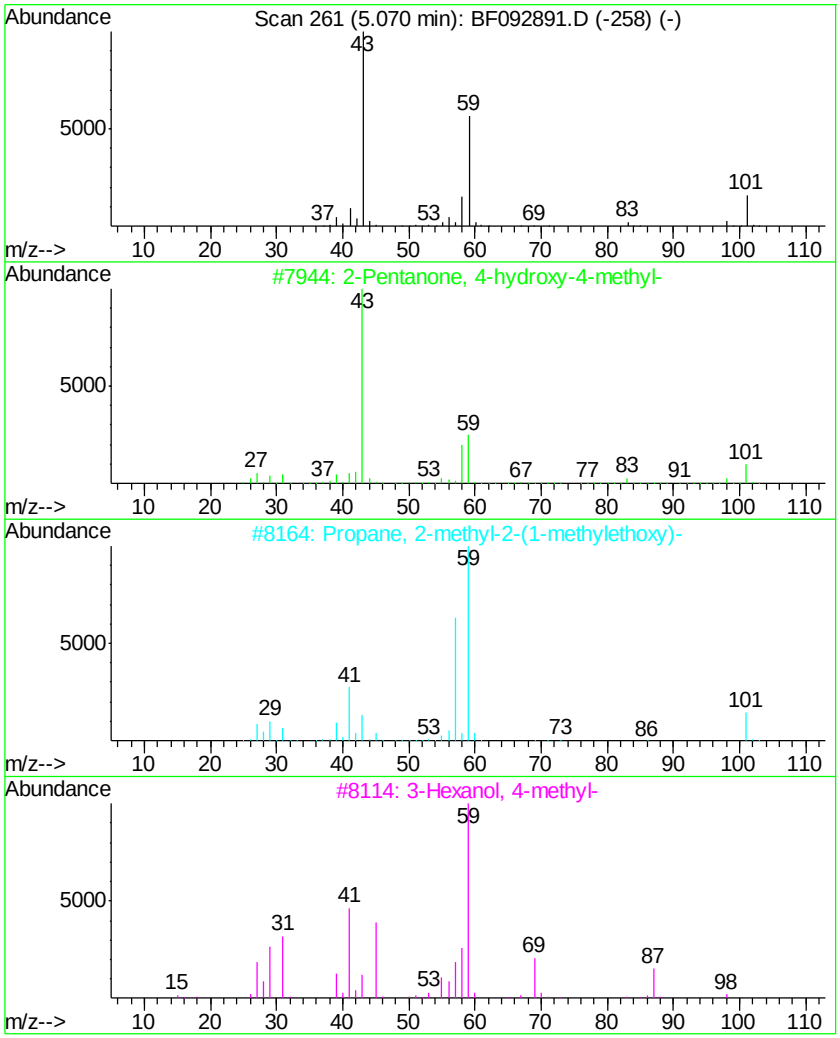
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

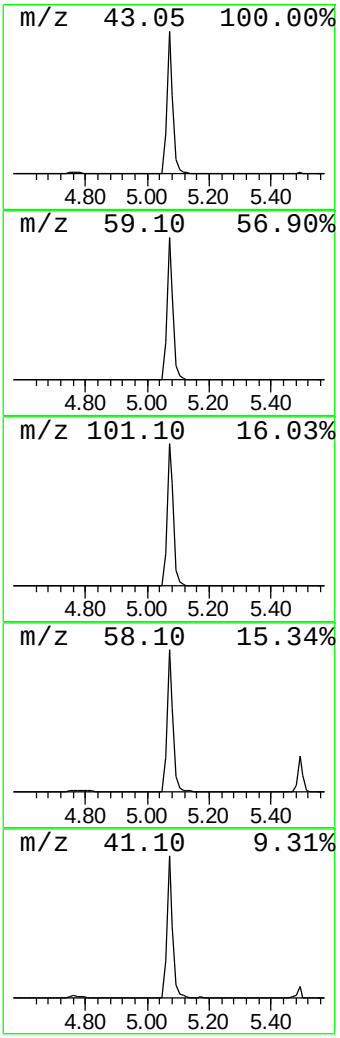
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	29.45 ng	1432370	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092891.D
Acq On : 10 Feb 2017 19:01
Operator : SJ/MA
Sample : I1777-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-11-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

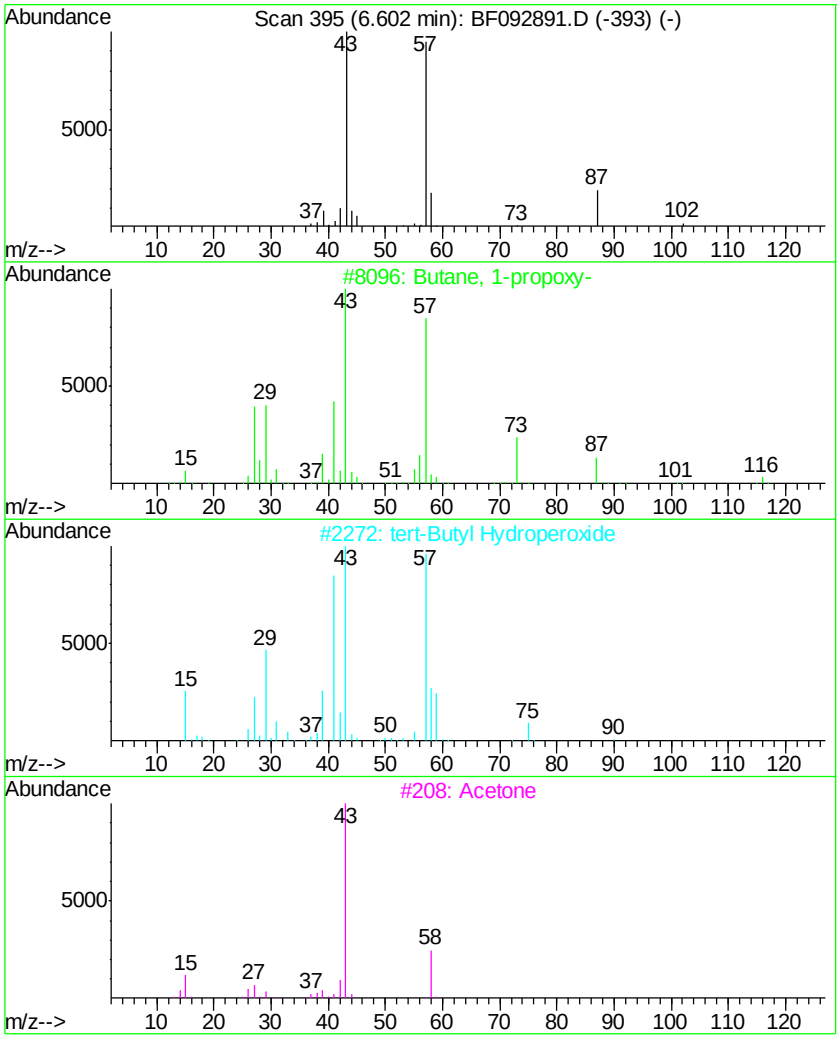
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

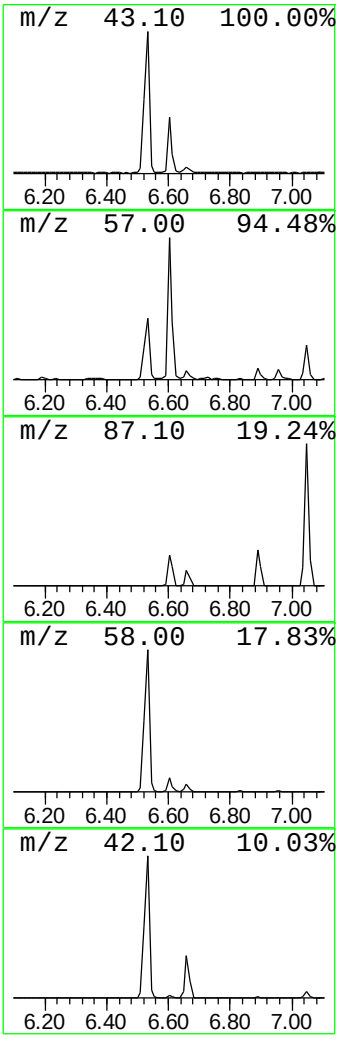
****

Peak Number 2 unknown6.60 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	2.55 ng	124093	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-propoxy-	116	C7H16O	003073-92-5	40
2	tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	33
3	Acetone	58	C3H6O	000067-64-1	25
4	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	23
5	2-Hydroxy-gamma-butyrolactone	102	C4H6O3	019444-84-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092891.D
Acq On : 10 Feb 2017 19:01
Operator : SJ/MA
Sample : I1777-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-11-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

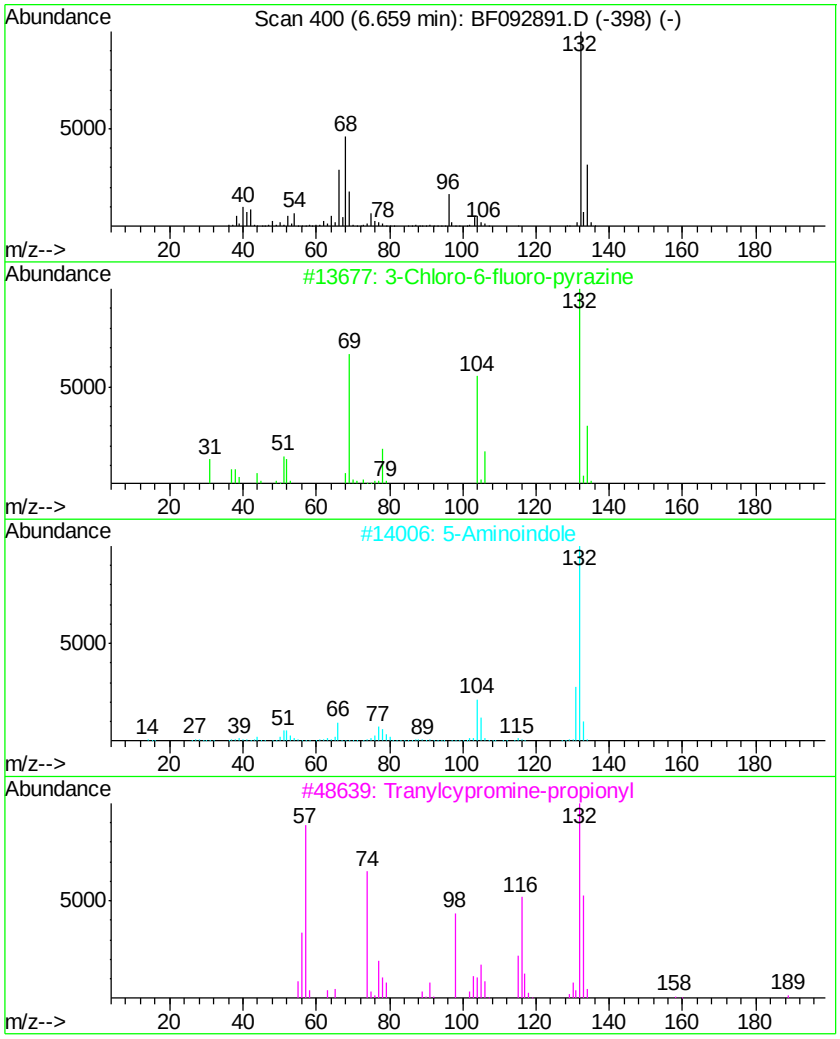
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

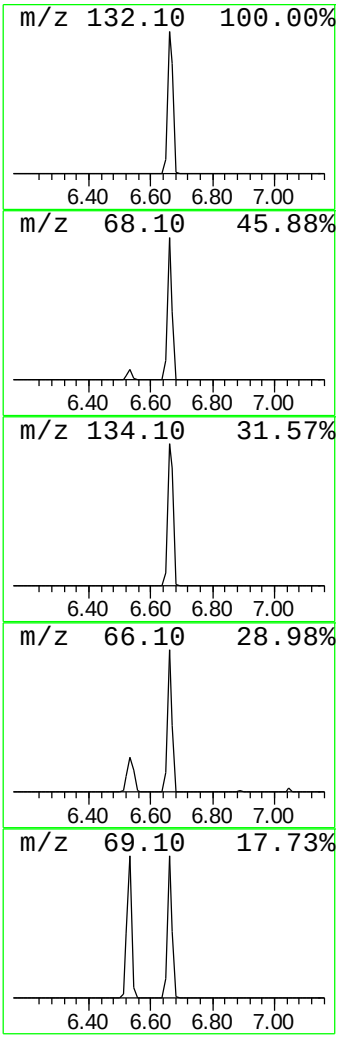
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	70.64 ng	3435340	1,4-Dichlorobenzene-d4	6.89

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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Operator : SJ/MA
Sample : I1777-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-11-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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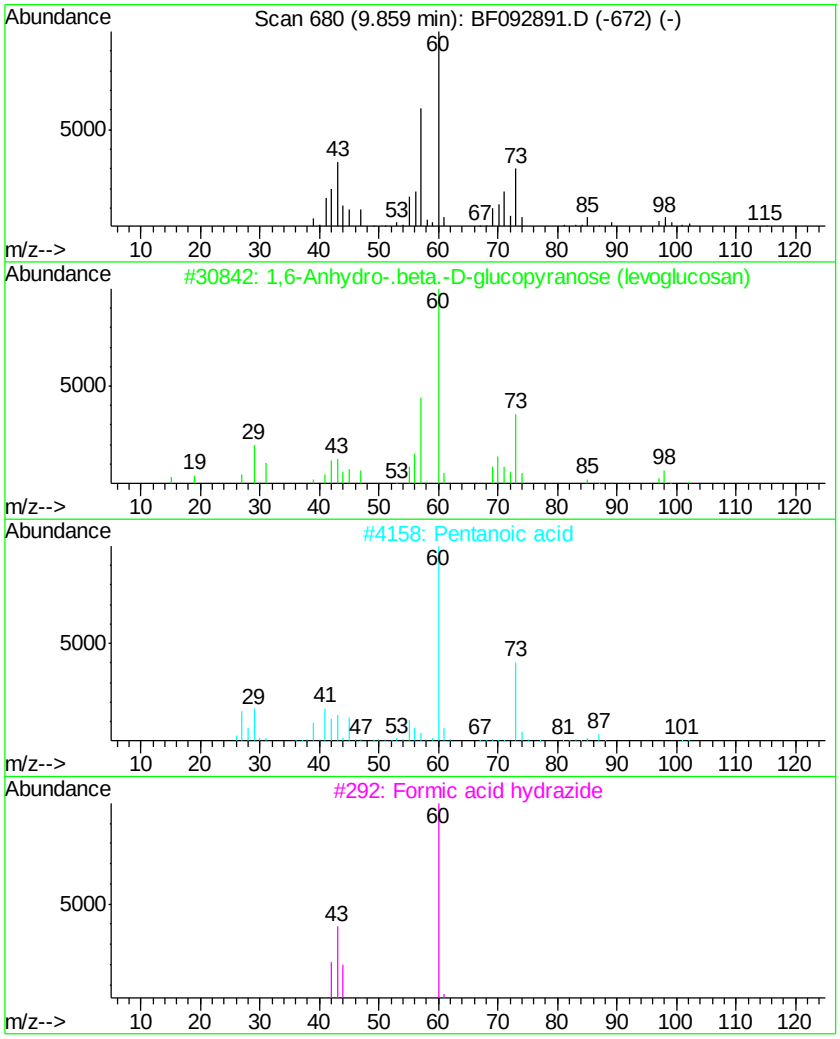
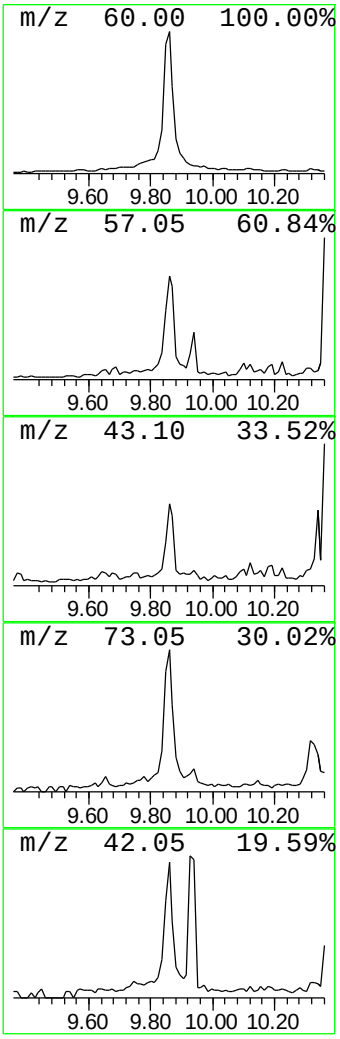
Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	3.81 ng	325714	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	64
2	Pentanoic acid	102	C5H10O2	000109-52-4	47
3	Formic acid hydrazide	60	CH4N2O	000624-84-0	43
4	Heptanoic acid	130	C7H14O2	000111-14-8	40
5	3,4-Altrosan	162	C6H10O5	1000129-76-4	40





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : 38-SB-03-11-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

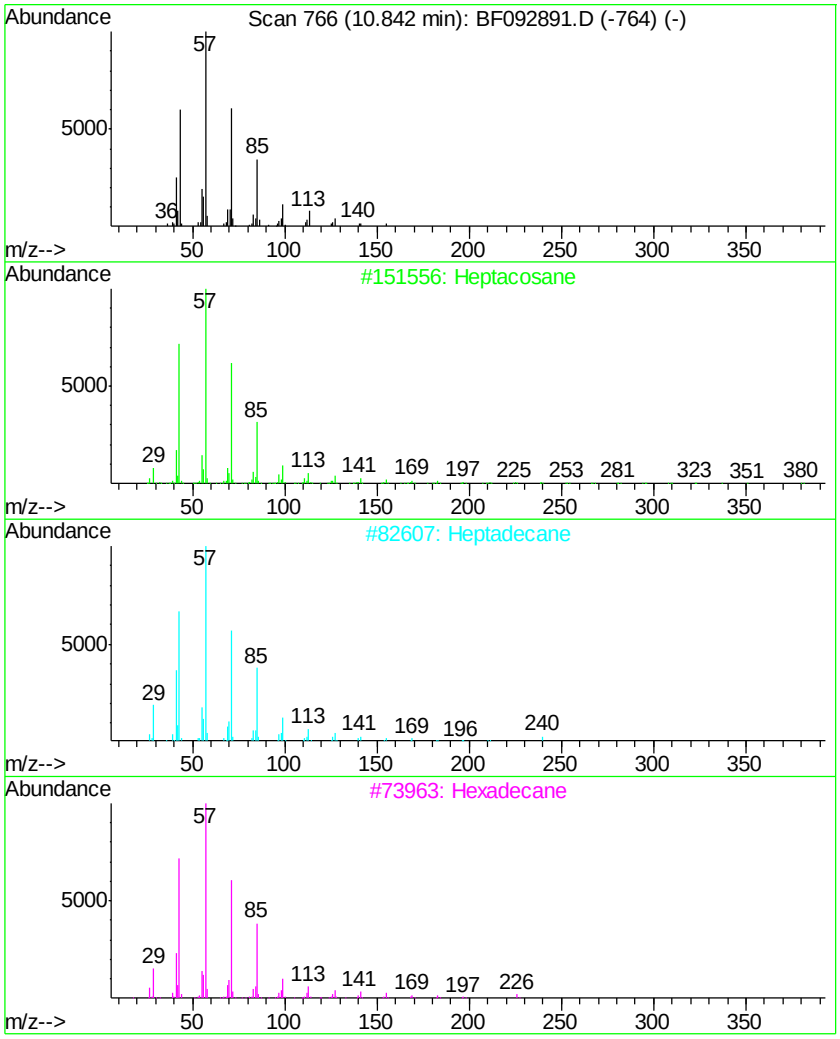
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

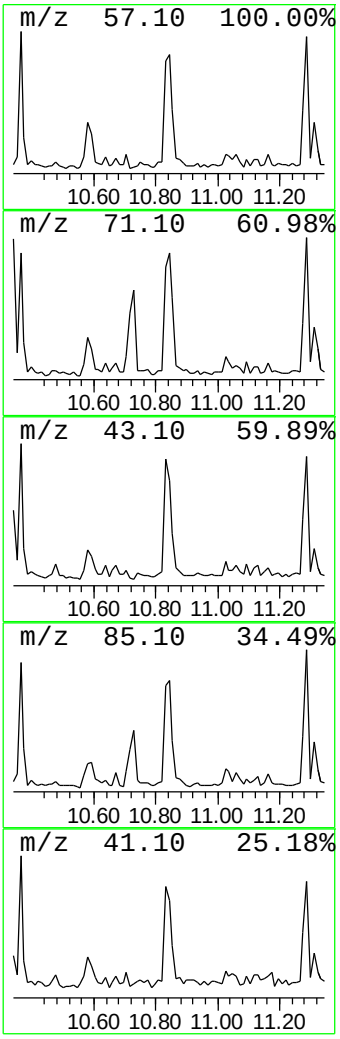
****

Peak Number 6 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.43 ng	192207	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Hexadecane	226	C16H34	000544-76-3	83
4	Pentadecane	212	C15H32	000629-62-9	80
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	74





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Sample : I1777-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-11-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

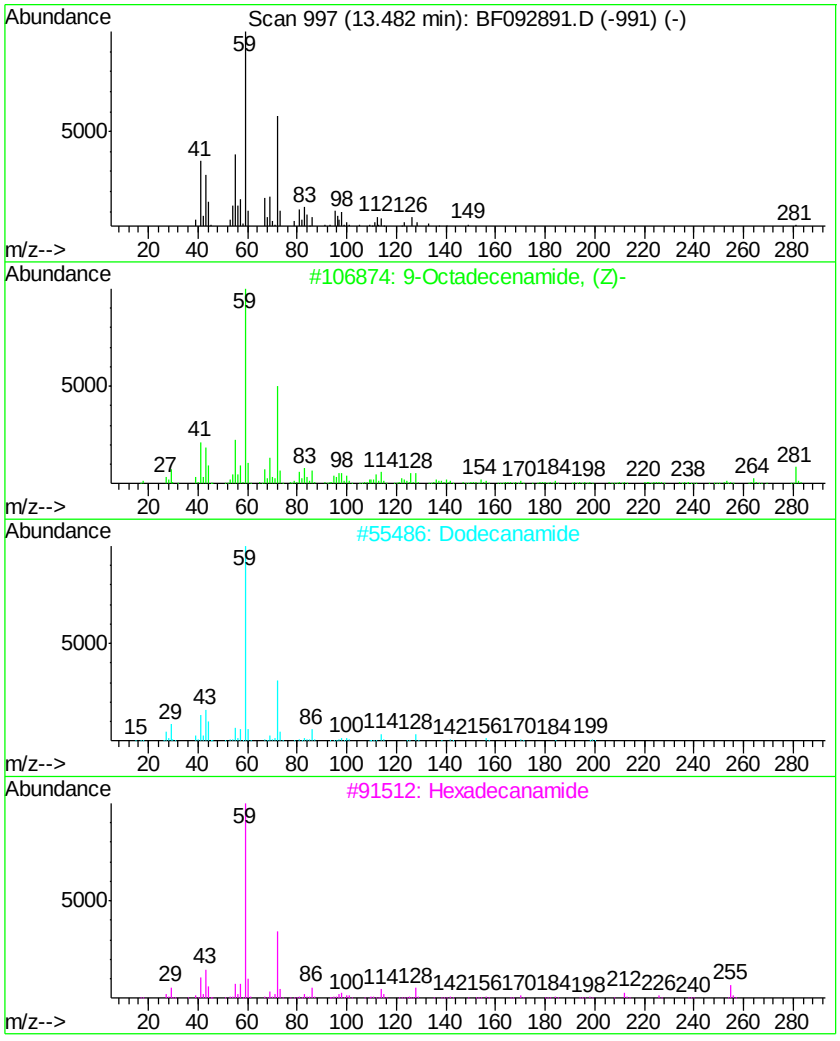
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

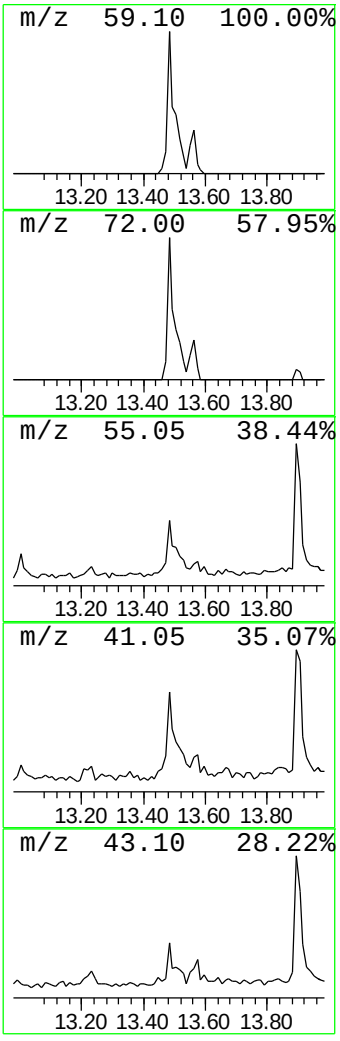
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.20 ng	145033	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Dodecanamide	199	C12H25NO	001120-16-7	59
3	Hexadecanamide	255	C16H33NO	000629-54-9	56
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

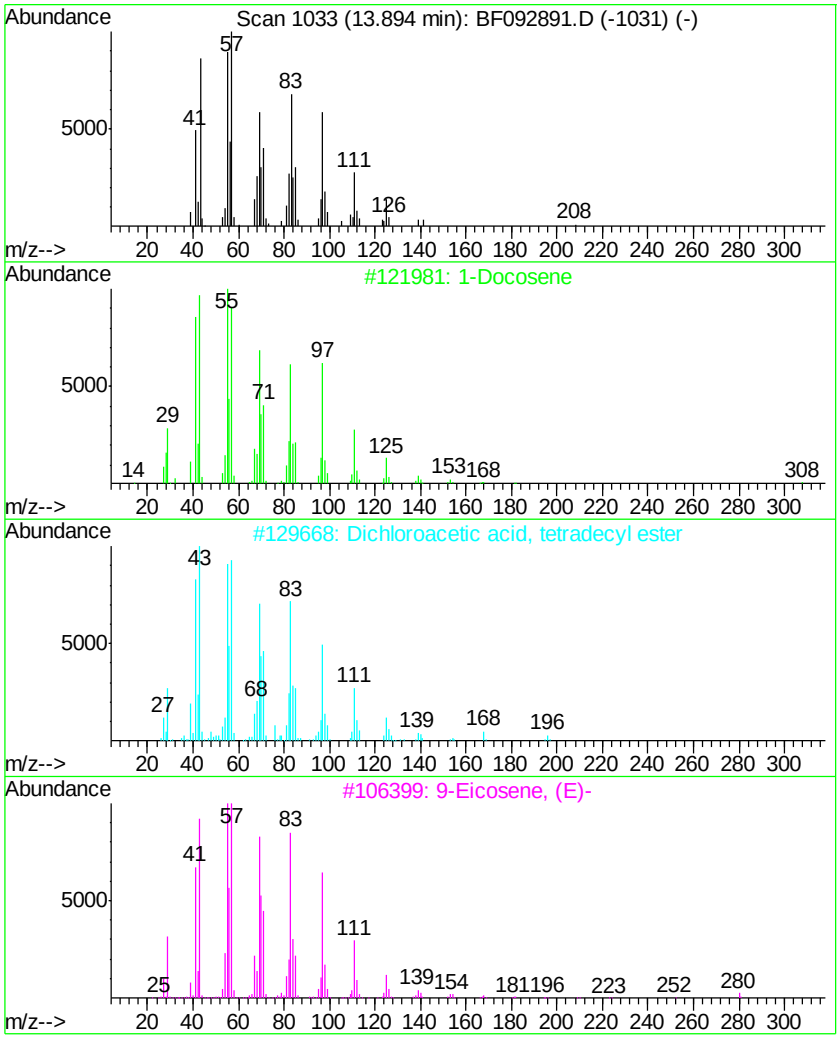
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

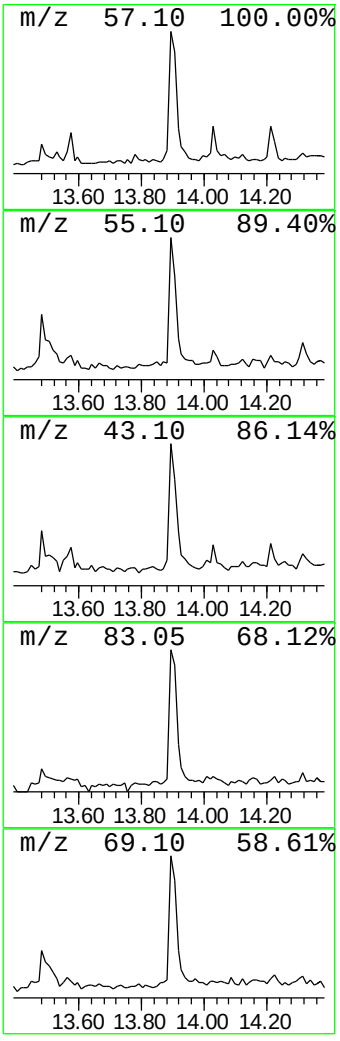
****

Peak Number 8 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.73 ng	179548	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	90
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	86





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.07	29.4	ng	1432370	1	6.89	972608	20.0
unknown6.60	6.60	2.5	ng	124093	1	6.89	972608	20.0
unknown6.66	6.66	70.6	ng	3435340	1	6.89	972608	20.0
1,6-Anhydro-.beta...	9.86	3.8	ng	325714	3	9.94	1710300	20.0
Heptacosane	10.84	2.4	ng	192207	4	11.42	1583410	20.0
9-Octadecenamide,...	13.48	2.2	ng	145033	5	14.05	1315810	20.0
1-Docosene	13.89	2.7	ng	179548	5	14.05	1315810	20.0