LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084239.D
Acq On : 4 Jan 2016 15:22
Operator : UM/SJ
Sample : G4981-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S8-0533

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-BF123115.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	4.430	203	205	209	rBV	240170	271434	2.44%	0.341%
2	5.081	260	262	271	rVB	1026490	1217144	10.93%	1.528%
3	5.504	296	299	301	rBV	4568855	5848715	52.53%	7.342%
4	6.522	386	388	391	rVB	3449644	3352993	30.11%	4.209%
5	6.659	397	400	403	rBV	7790701	8093424	72.69%	10.159%
6	6.887	418	420	423	rBV	2657271	2217458	19.92%	2.783%
7	7.047	431	434	436	rBV	8249933	7502727	67.38%	9.418%
8	7.459	466	470	472	rBV	6608002	7129463	64.03%	8.949%
9	7.687	488	490	491	rVB	319098	228321	2.05%	0.287%
10	7.905	504	509	512	rBV2	87793	113374	1.02%	0.142%
11	8.179	530	533	535	rBV	2965273	2973403	26.70%	3.732%
12	9.253	624	627	630	rBV	8419624	11134409	100.00%	13.977%
13	9.653	659	662	663	rBV	796864	829376	7.45%	1.041%
14	9.928	684	686	689	rVB	2747935	2999046	26.93%	3.765%
15	10.362	721	724	726	rVB3	81194	145043	1.30%	0.182%
16	10.728	752	756	758	rBV	5098280	7257325	65.18%	9.110%
17	10.842	762	766	772	rVB2	115867	208976	1.88%	0.262%
18	11.311	803	807	809	rBV	812694	835857	7.51%	1.049%
19	11.413	814	816	819	rVB	3284685	2848486	25.58%	3.576%
20	12.831	938	940	942	rBV	533097	470549	4.23%	0.591%
21	12.899	942	946	948	rVB2	97311	129993	1.17%	0.163%
22	13.002	952	955	958	rBV	7043807	9591042	86.14%	12.039%
23	13.528	999	1001	1003	rBV2	201462	274926	2.47%	0.345%
24	13.905	1031	1034	1038	rBV	202965	263957	2.37%	0.331%
25	14.054	1044	1047	1049	rBV	1859007	2063667	18.53%	2.590%
26	15.494	1169	1173	1175	rBV	1075225	1663921	14.94%	2.089%

Sum of corrected areas: 79665029

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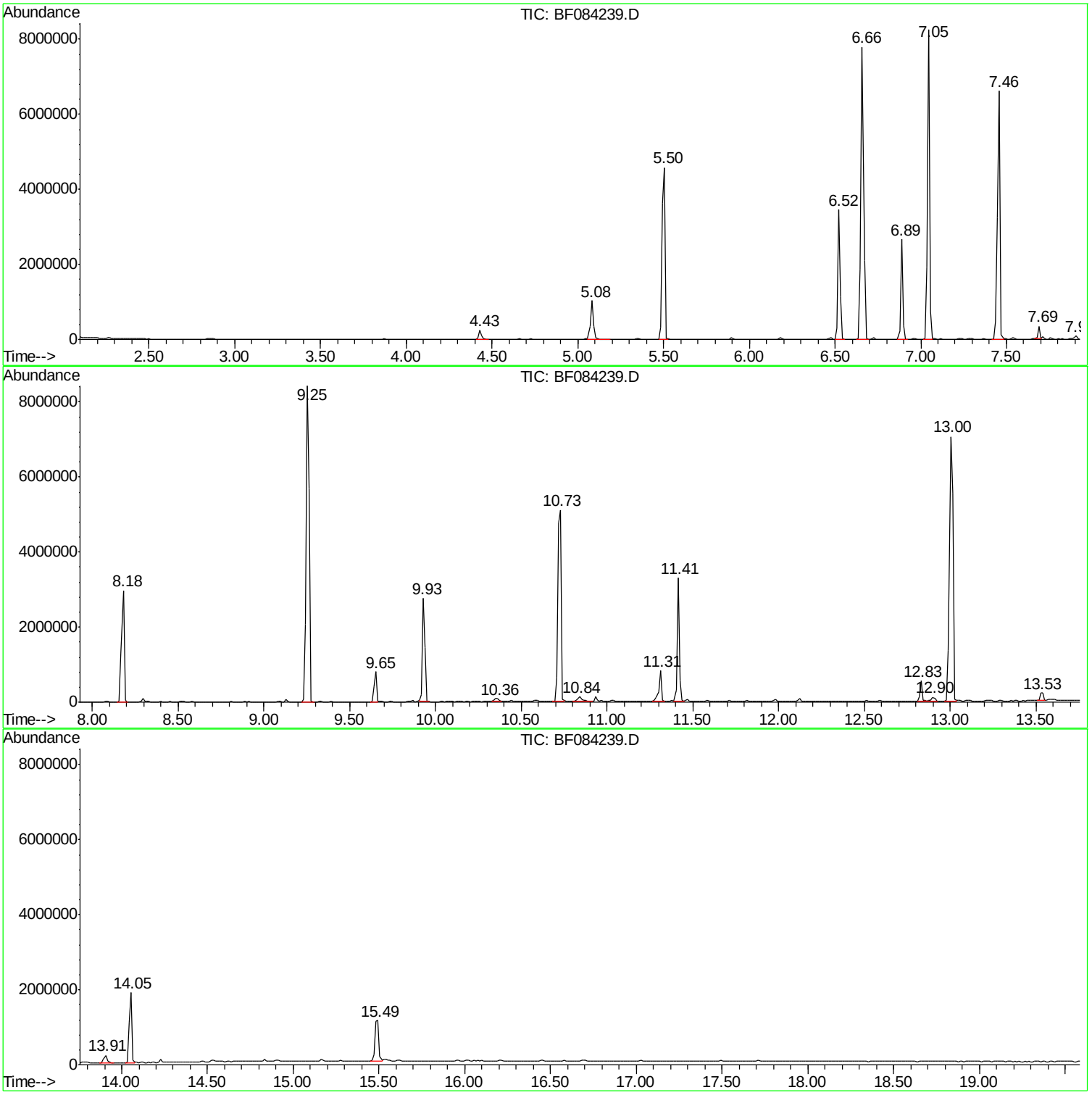
Instrument : BNA_F
ClientSampleId : S8-0533

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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Data File : BF084239.D
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Operator : UM/SJ
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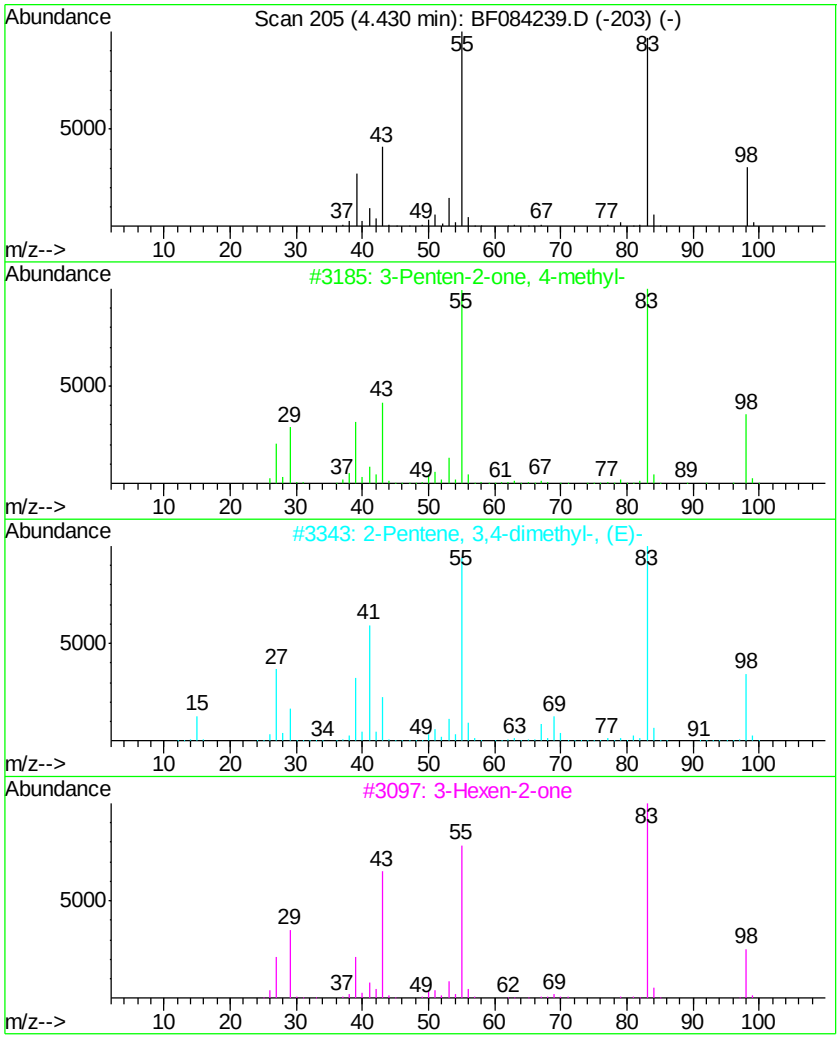
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

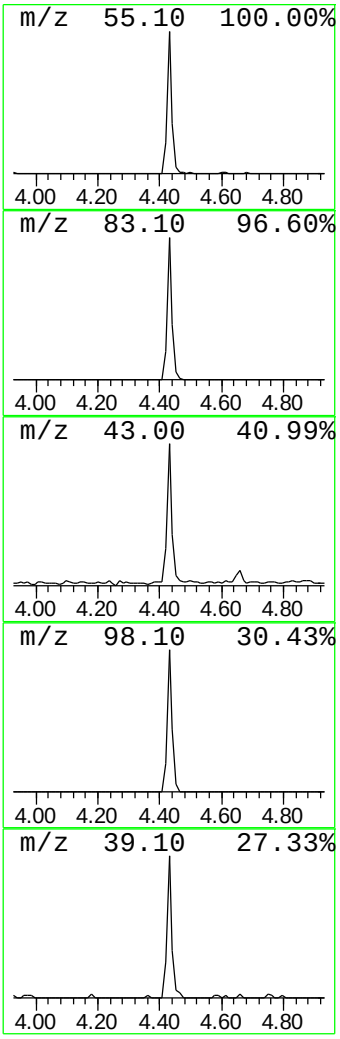
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	2.45 ng	271434	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





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Data File : BF084239.D
Acq On : 4 Jan 2016 15:22
Operator : UM/SJ
Sample : G4981-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S8-0533

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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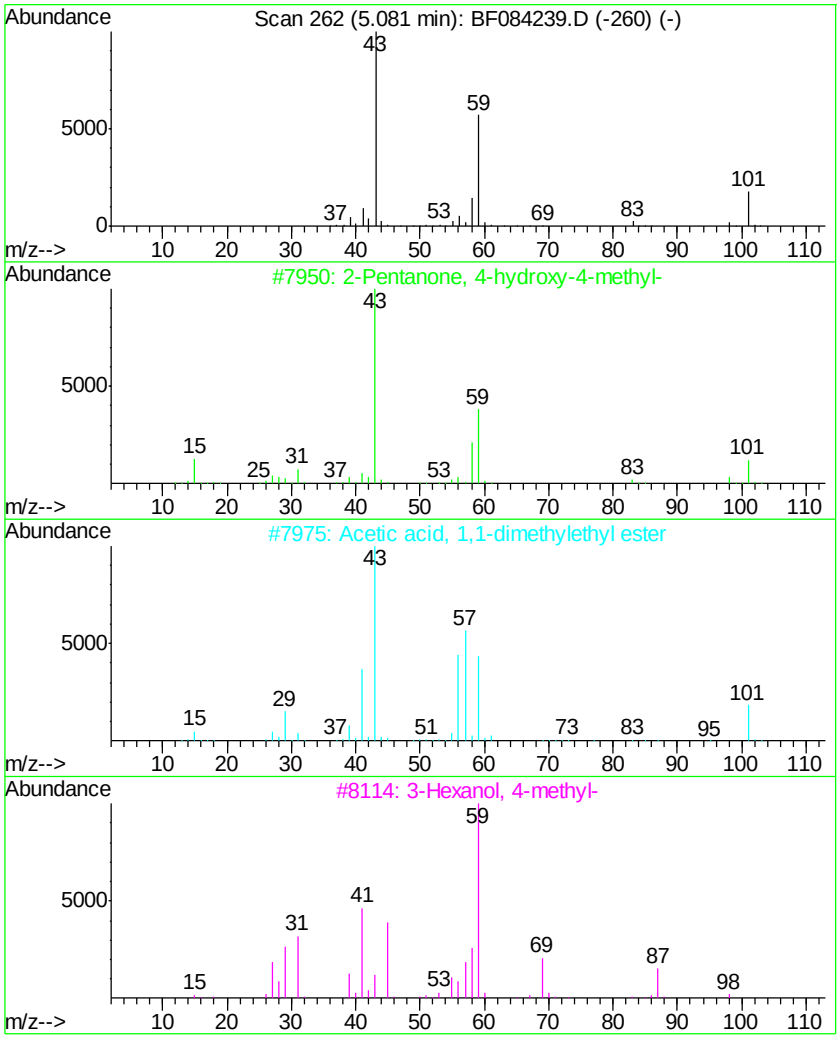
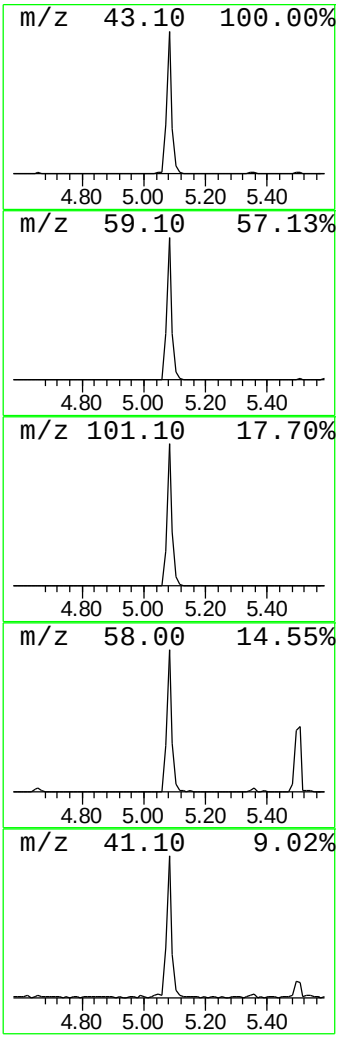
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	10.98 ng	1217140	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	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084239.D
Acq On : 4 Jan 2016 15:22
Operator : UM/SJ
Sample : G4981-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S8-0533

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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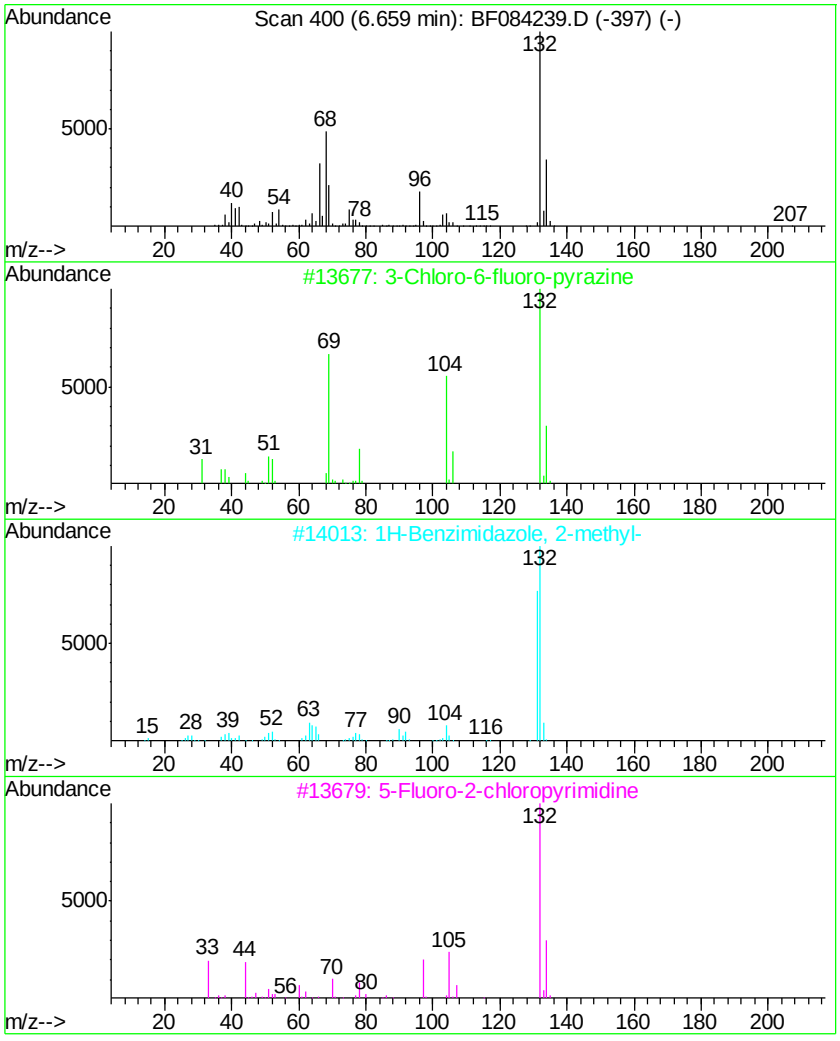
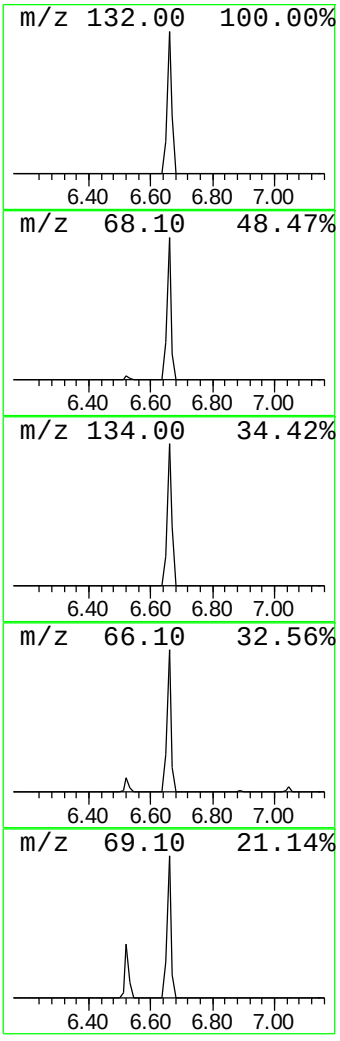
Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	73.00 ng	8093420	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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9





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Data File : BF084239.D
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Operator : UM/SJ
Sample : G4981-06
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S8-0533

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

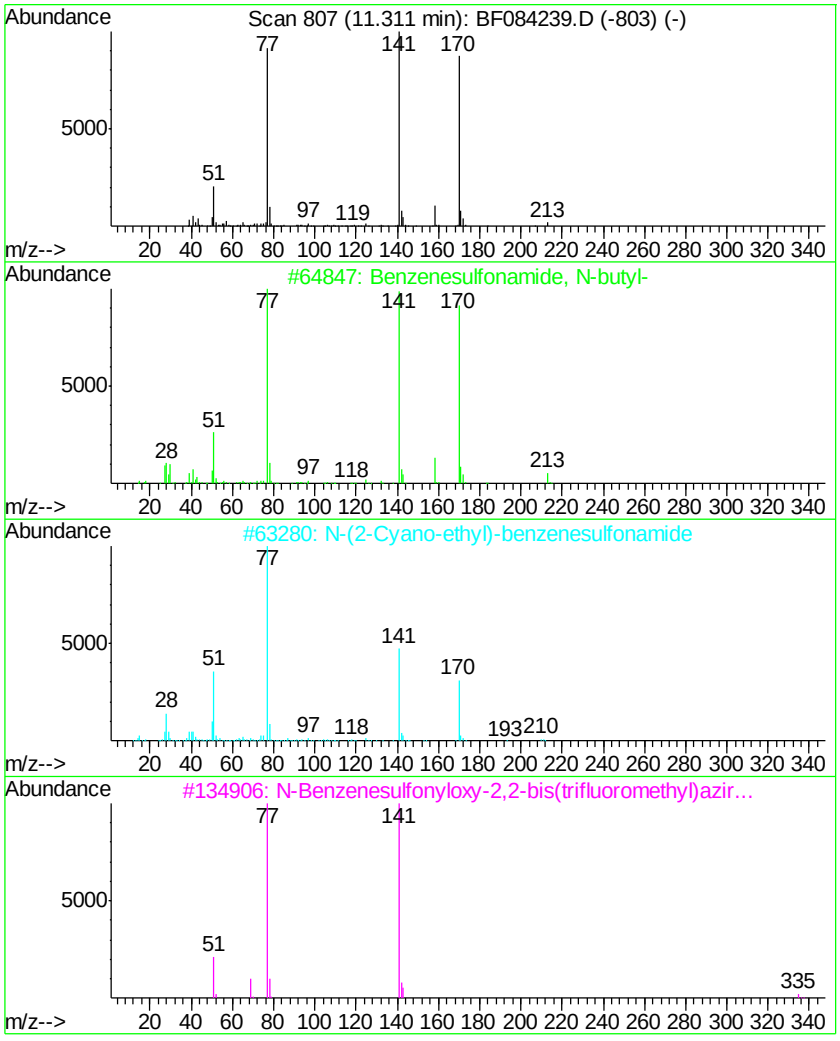
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

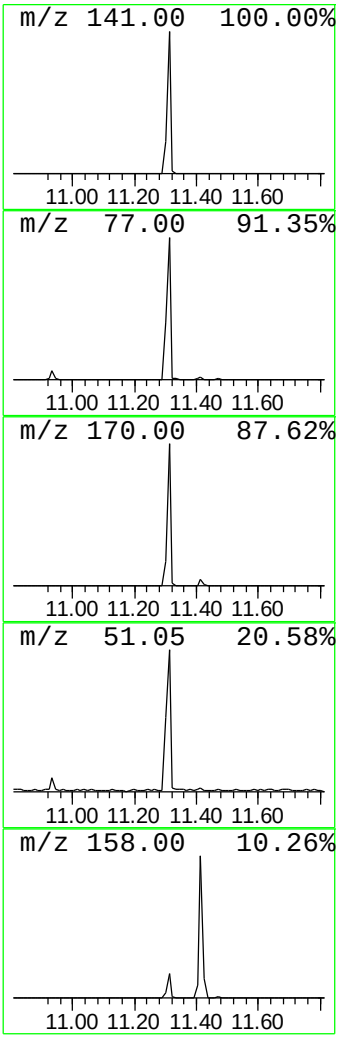
****

Peak Number 5 Benzenesulfonamide, N-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.31	5.87 ng	835857	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	91
2	N-(2-Cyano-ethyl)-benzenesulfona...	210	C9H10N2O2S	002619-21-8	83
3	N-Benzenesulfonyloxy-2,2-bis(tri...	335	C10H7F6NO3S	055734-41-3	50
4	(Phenylsulfonyl)acetonitrile	181	C8H7NO2S	007605-28-9	47
5	N,N-Dichlorobenzenesulfonamide	225	C6H5Cl2NO2S	000473-29-0	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084239.D
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Operator : UM/SJ
Sample : G4981-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S8-0533

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

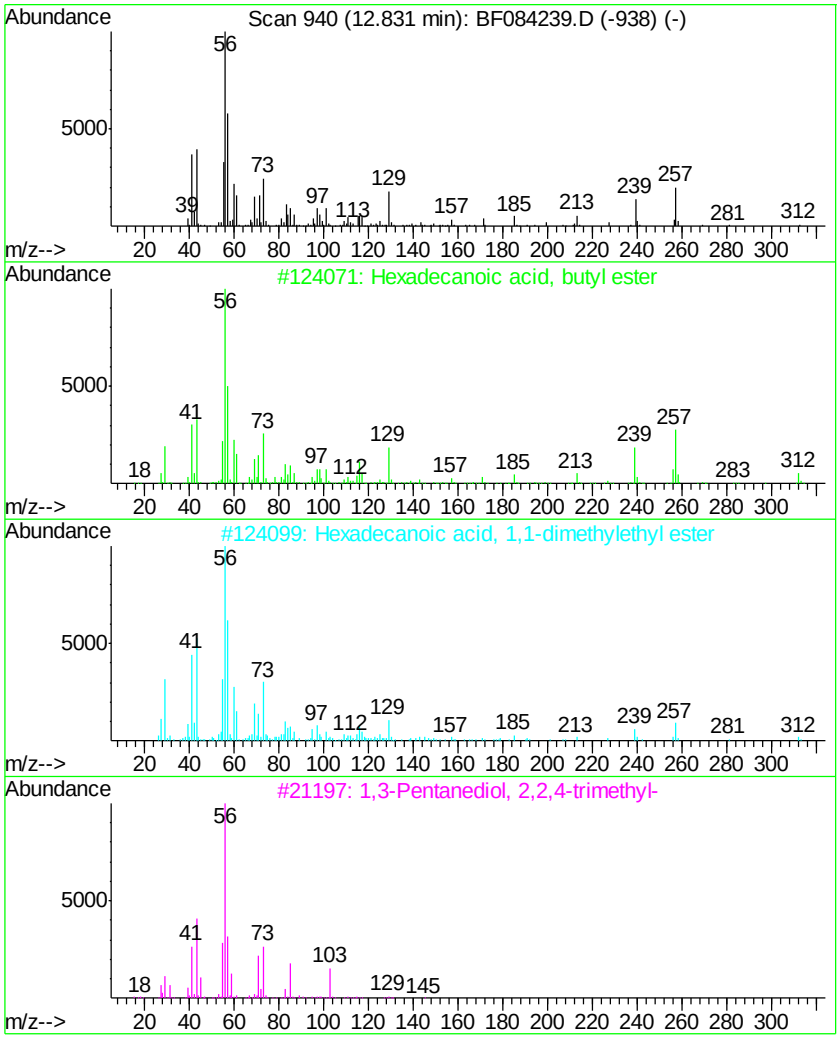
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

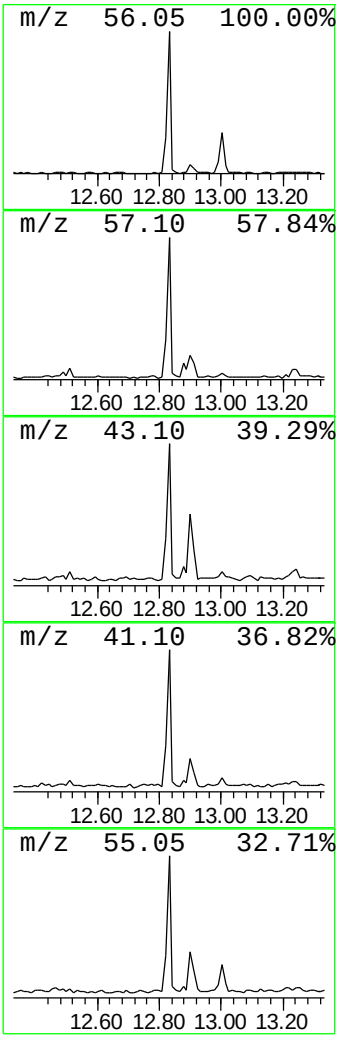
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	4.56 ng	470549	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	43
4	Cyclopentanamine	85	C5H11N	001003-03-8	35
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35





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Instrument : BNA_F
ClientSampleId : S8-0533

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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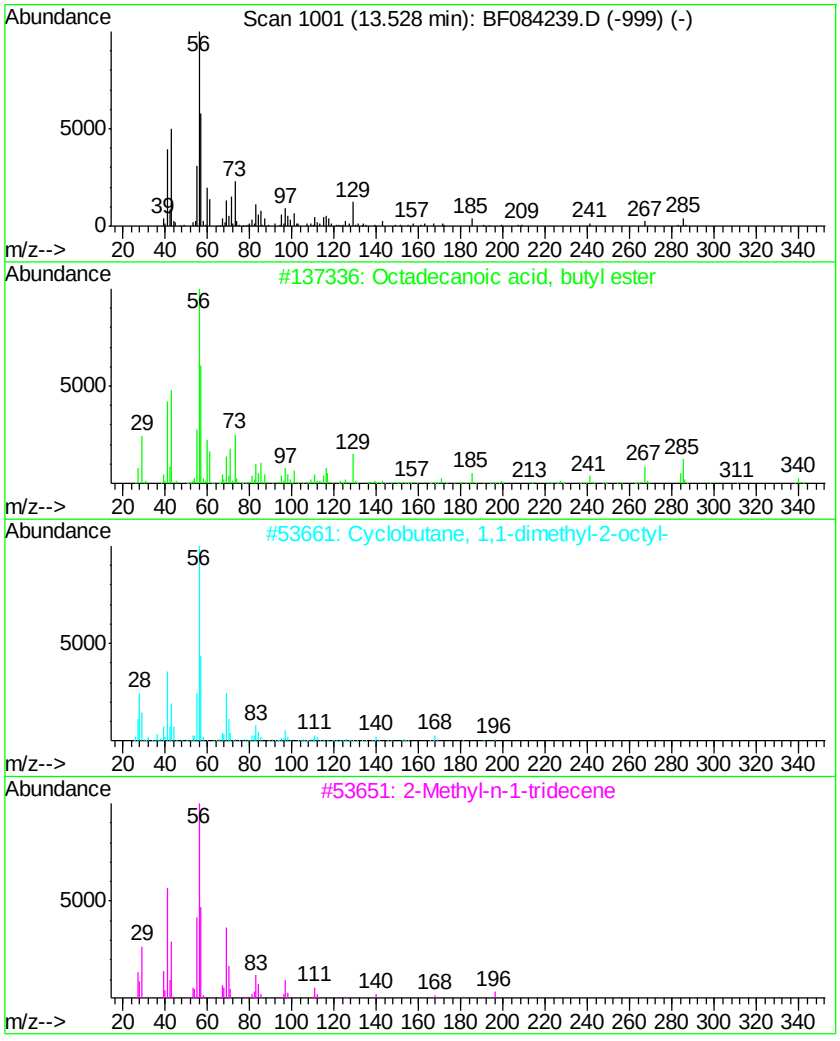
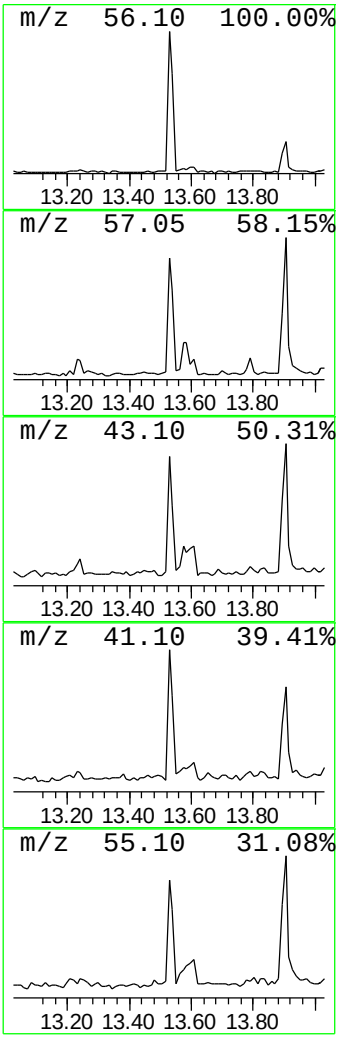
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.66 ng	274926	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
3	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35





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Instrument : BNA_F
ClientSampleId : S8-0533

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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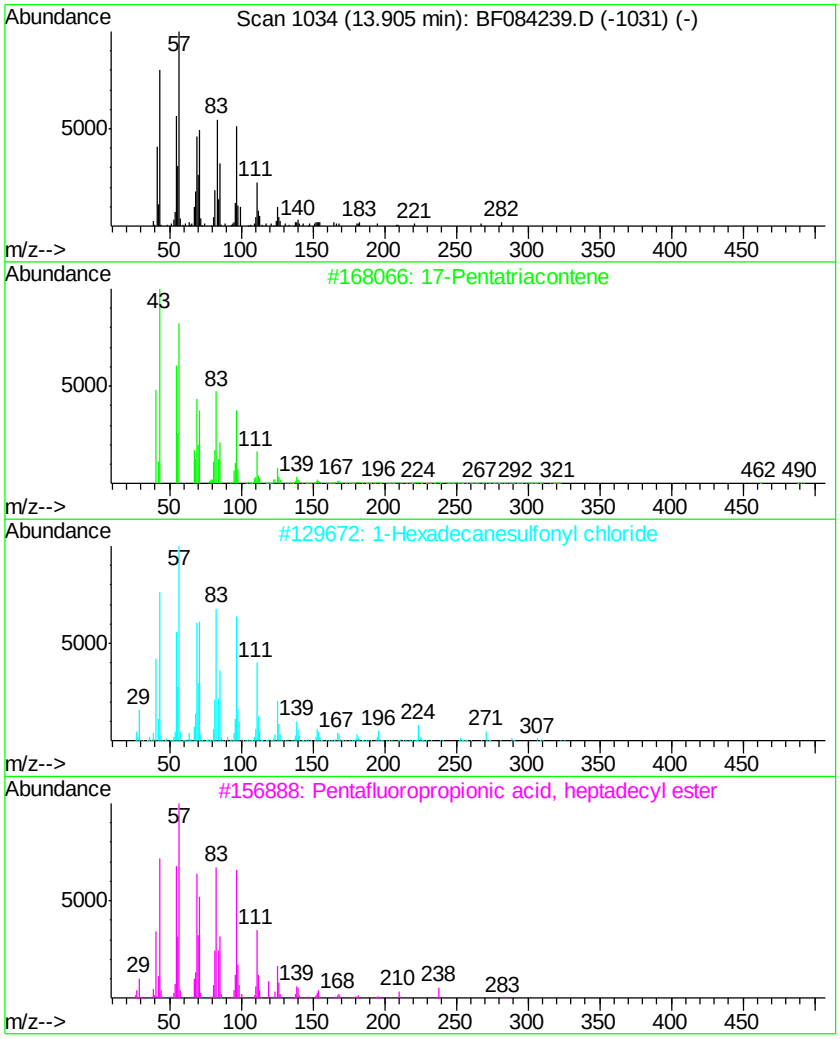
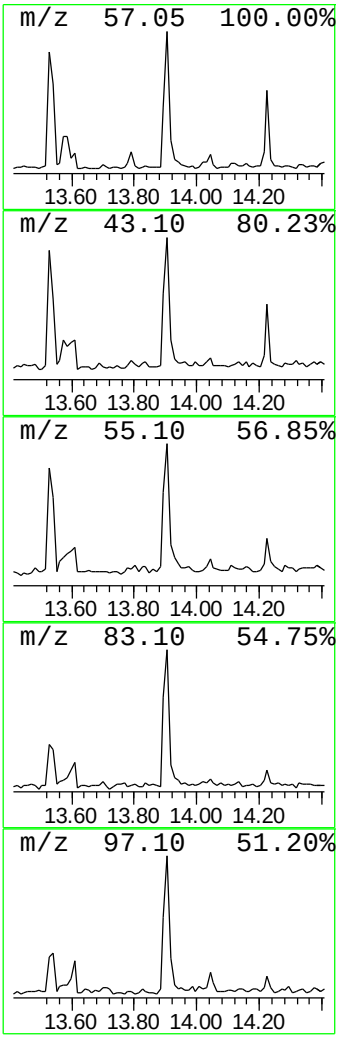
Peak Number 8 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	2.56 ng	263957	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	86
4	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	80
5	1-Nonadecene	266	C19H38	018435-45-5	74





Tentatively Identified Compound (LSC) summary

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Operator : UM/SJ
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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
3-Penten-2-one, 4...	4.43	2.5	ng	271434	1	6.89	2217460	20.0
2-Pentanone, 4-hy...	5.08	11.0	ng	1217140	1	6.89	2217460	20.0
unknown6.66	6.66	73.0	ng	8093420	1	6.89	2217460	20.0
Benzenesulfonamid...	11.31	5.9	ng	835857	4	11.41	2848490	20.0
Hexadecanoic acid...	12.83	4.6	ng	470549	5	14.05	2063670	20.0
Octadecanoic acid...	13.53	2.7	ng	274926	5	14.05	2063670	20.0
17-Pentatriacontene	13.91	2.6	ng	263957	5	14.05	2063670	20.0