LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081760.D
Acq On : 23 Sep 2015 7:41
Operator : UM/IZ
Sample : G3748-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP205-17-19

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-BF090115.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	1.258	10	15	17	rBV	1001575	1290852	69.08%	6.993%
2	1.430	29	30	36	rBV	104400	275104	14.72%	1.490%
3	1.521	36	38	72	rVB	499520	1734444	92.82%	9.396%
4	4.436	289	293	316	rBV	273239	932629	49.91%	5.052%
5	5.316	366	370	396	rBV	868575	1690564	90.48%	9.158%
6	7.579	564	568	571	rBV	792538	1655723	88.61%	8.969%
7	7.659	571	575	584	rVB	1001827	1868517	100.00%	10.122%
8	8.127	613	616	623	rVB	157487	277132	14.83%	1.501%
9	8.459	641	645	648	rBV	710104	1229610	65.81%	6.661%
10	9.442	726	731	734	rBV	550071	1077470	57.66%	5.837%
11	11.031	866	870	883	rBV	202027	350993	18.78%	1.901%
12	13.682	1096	1102	1105	rBV	907082	1711177	91.58%	9.270%
13	14.734	1190	1194	1204	rBB	162675	265858	14.23%	1.440%
14	15.157	1227	1231	1238	rBB2	224383	377902	20.22%	2.047%
15	17.077	1394	1399	1410	rBB	552828	1120390	59.96%	6.069%
16	18.666	1534	1538	1545	rBV	228672	384602	20.58%	2.083%
17	20.426	1689	1692	1704	rBV2	24587	62092	3.32%	0.336%
18	21.969	1824	1827	1829	rVB	17907	19972	1.07%	0.108%
19	22.049	1831	1834	1837	rBV	1087702	1377897	73.74%	7.464%
20	22.883	1904	1907	1909	rBV	14149	19674	1.05%	0.107%
21	23.295	1940	1943	1944	rBV2	83521	94422	5.05%	0.512%
22	23.329	1944	1946	1953	rVV	274582	302919	16.21%	1.641%
23	24.255	2025	2027	2029	rBV	66010	72398	3.87%	0.392%
24	24.346	2033	2035	2037	rVB	25259	22041	1.18%	0.119%
25	24.769	2070	2072	2076	rBV	186390	201138	10.76%	1.090%
26	25.192	2107	2109	2115	rVB3	11239	21408	1.15%	0.116%
27	25.935	2171	2174	2184	rVB3	5702	22848	1.22%	0.124%

Sum of corrected areas: 18459776

LSC Report - Integrated Chromatogram

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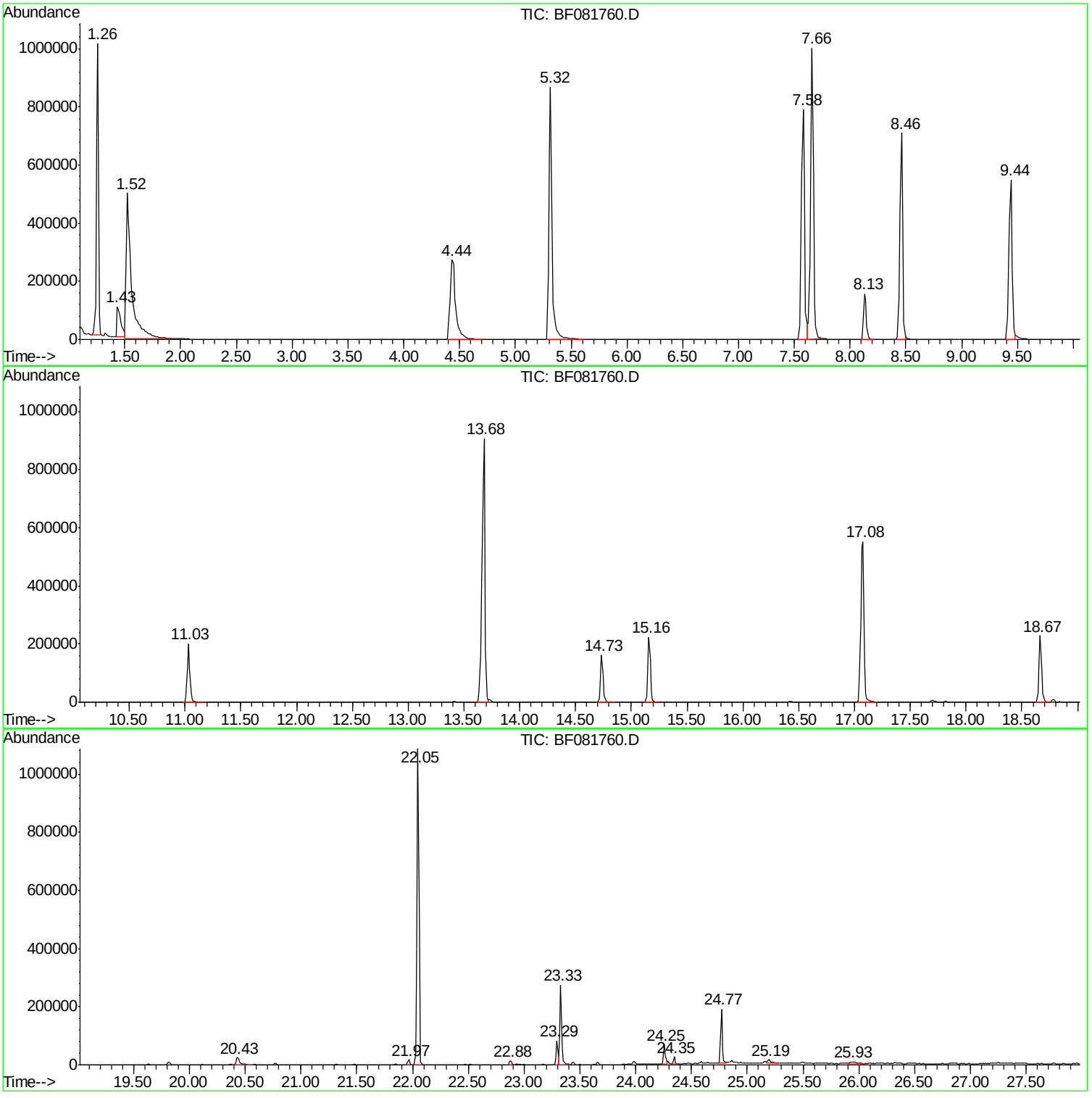
Operator : UM/IZ
Sample : G3748-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP205-17-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081760.D
Acq On : 23 Sep 2015 7:41
Operator : UM/IZ
Sample : G3748-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP205-17-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

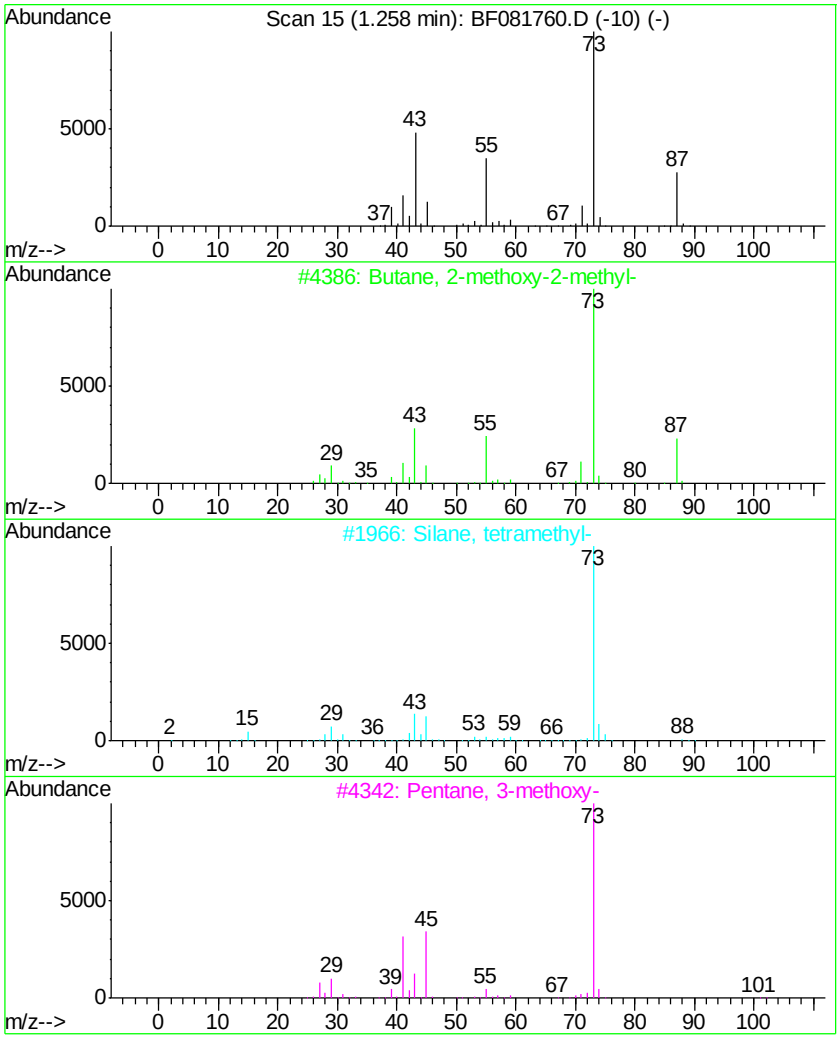
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

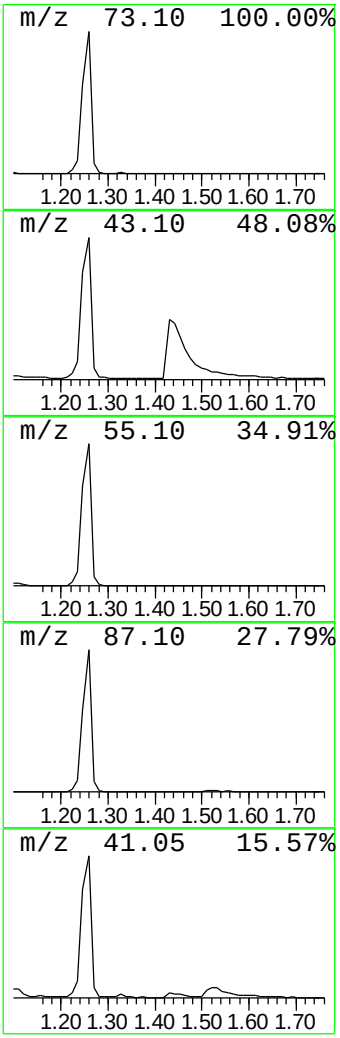
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	93.16 ng	1290850	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081760.D
Acq On : 23 Sep 2015 7:41
Operator : UM/IZ
Sample : G3748-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP205-17-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

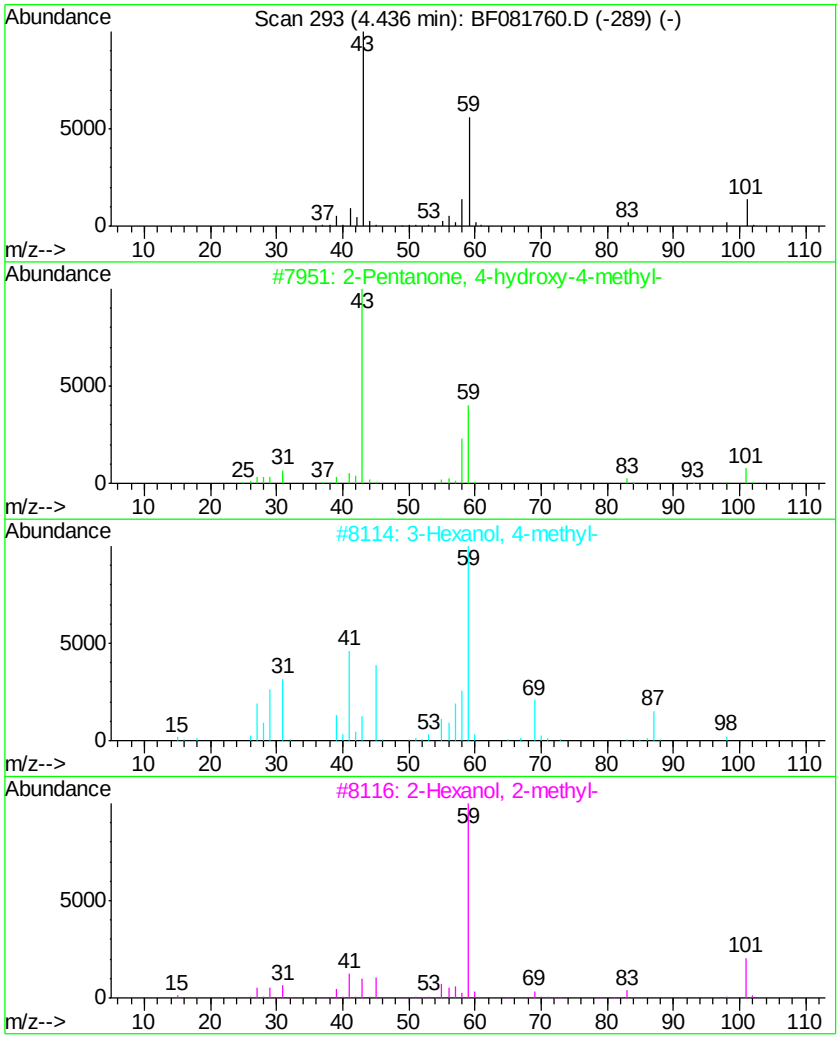
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

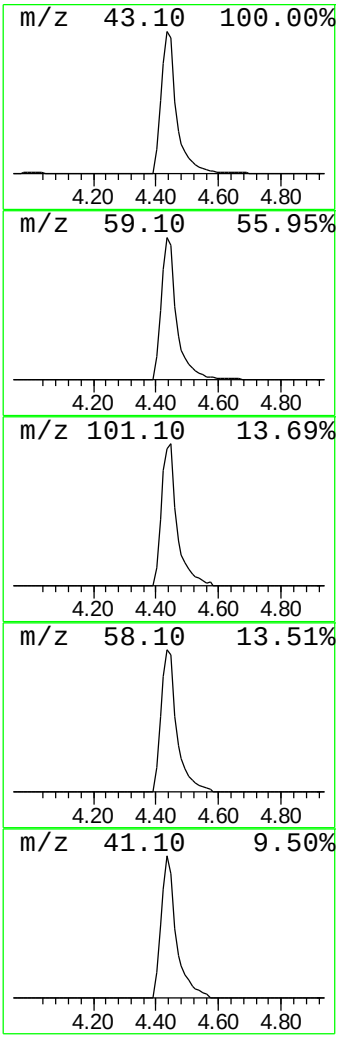
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	67.31 ng	932629	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081760.D
Acq On : 23 Sep 2015 7:41
Operator : UM/IZ
Sample : G3748-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP205-17-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

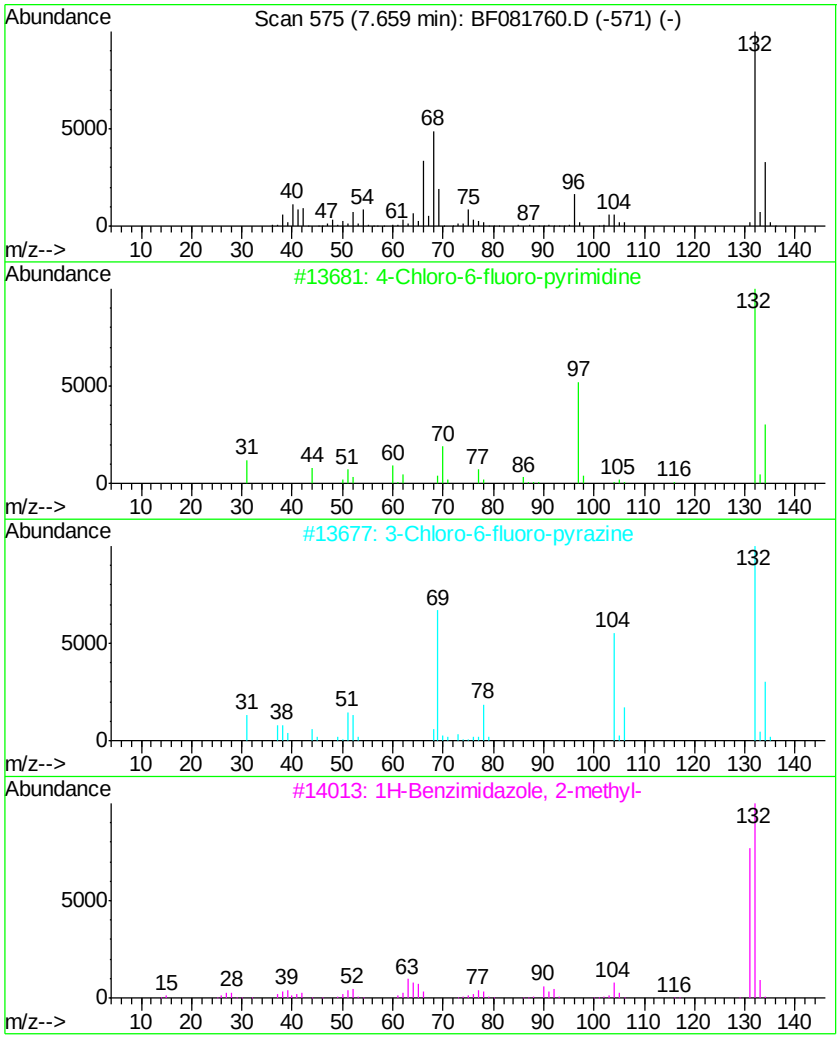
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

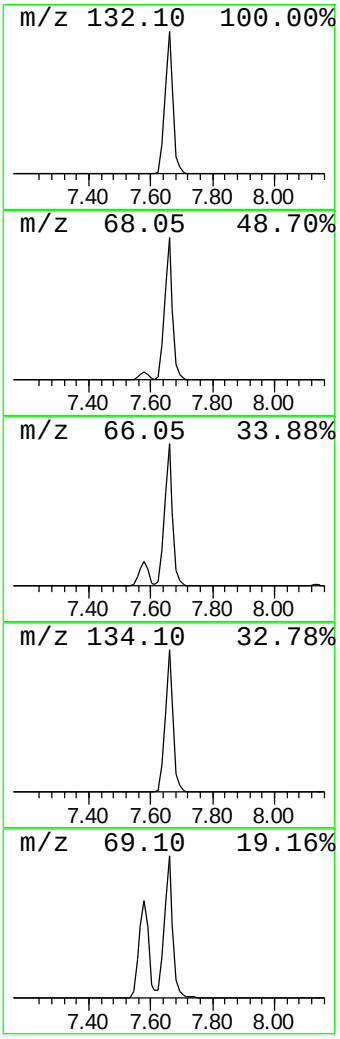
****

Peak Number 5 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	134.85 ng	1868520	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
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Sample : G3748-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP205-17-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

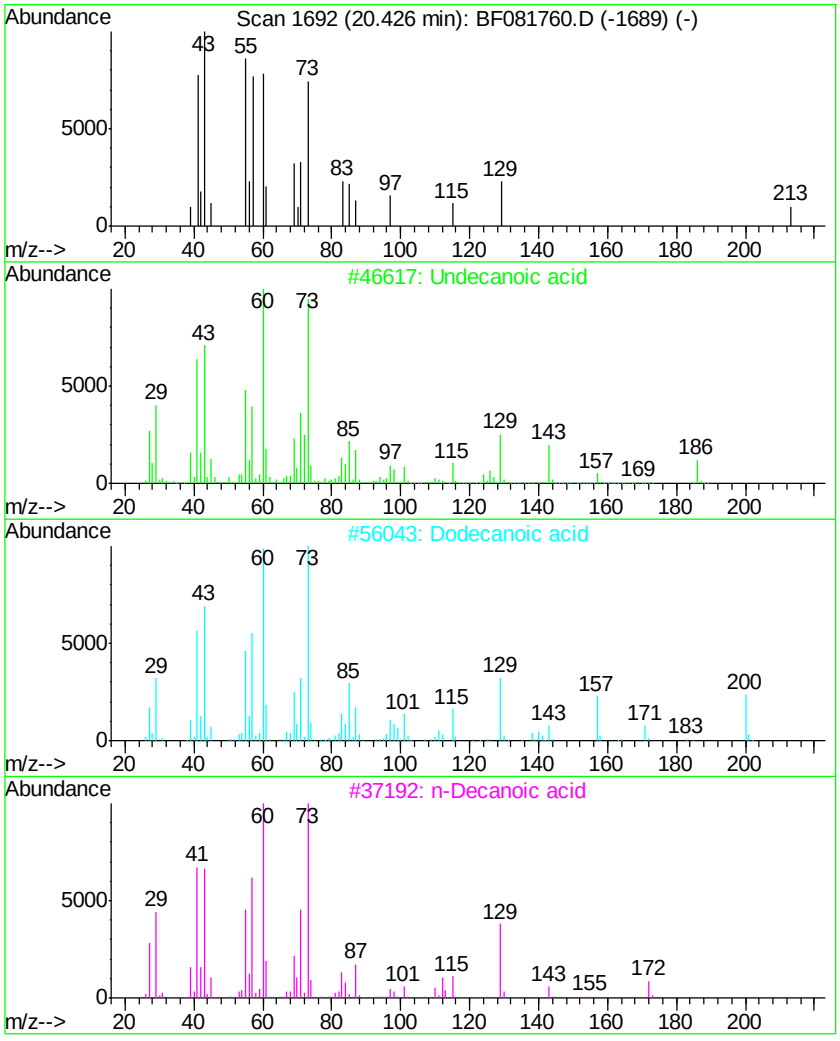
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

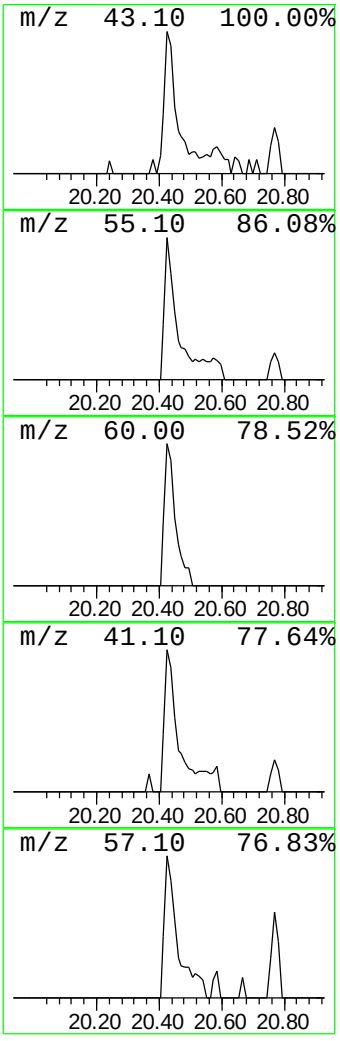
****

Peak Number 7 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	3.23 ng	62092	Phenanthrene-d10	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	Dodecanoic acid	200	C12H24O2	000143-07-7	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	50
5	Amyl Nitrite	117	C5H11NO2	000110-46-3	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081760.D
Acq On : 23 Sep 2015 7:41
Operator : UM/IZ
Sample : G3748-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP205-17-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

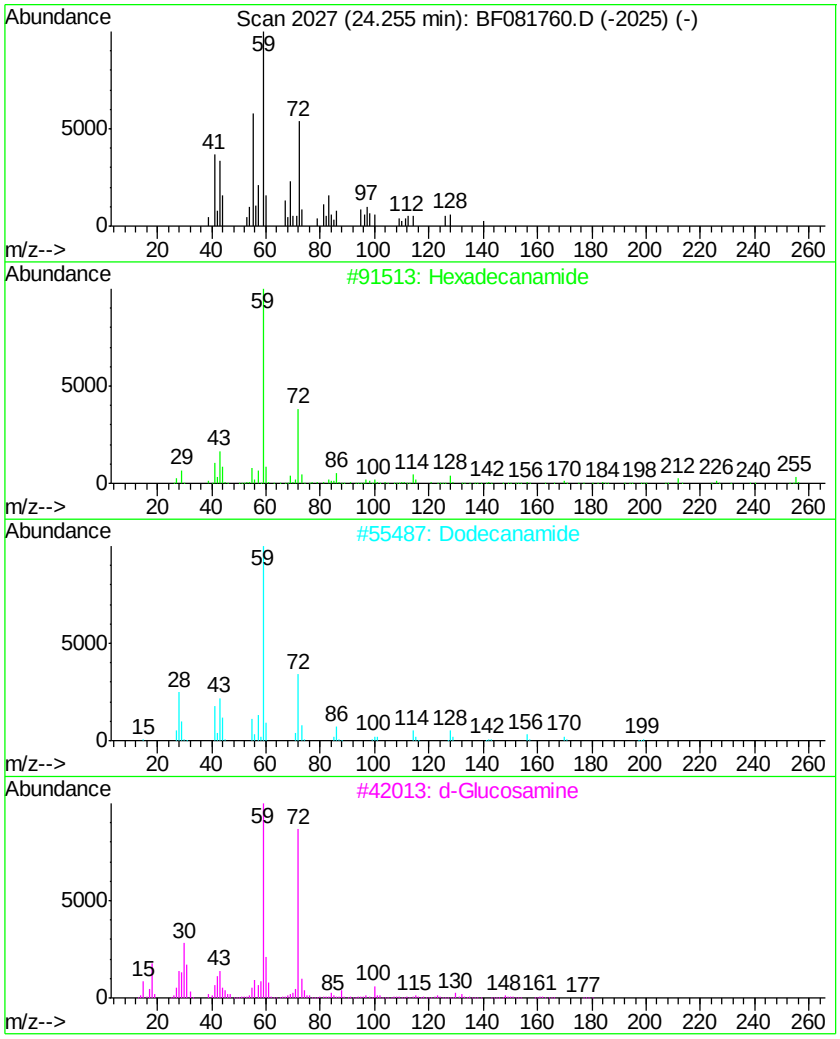
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

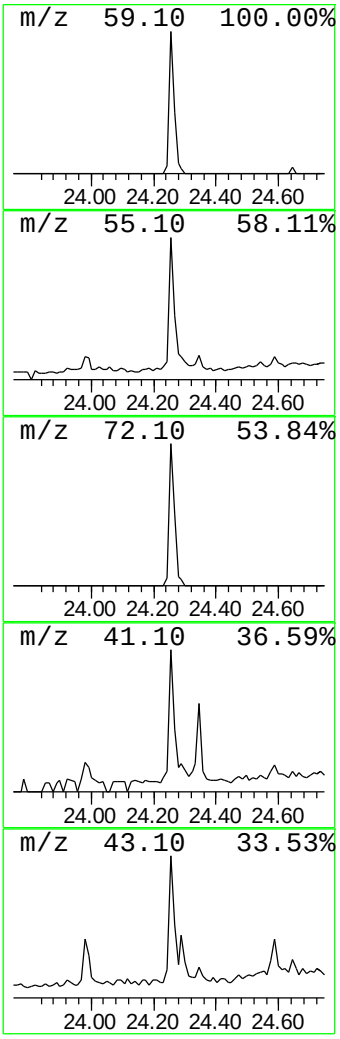
****

Peak Number 8 Hexadecanamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.25	7.20 ng	72398	Perylene-d12	24.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	50
2	Dodecanamide	199	C12H25NO	001120-16-7	50
3	d-Glucosamine	179	C6H13NO5	000090-77-7	45
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	45
5	2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	43





Library Search Compound Report

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Sample : G3748-05
Misc :
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Instrument : BNA_F
ClientSampleId : MGP205-17-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

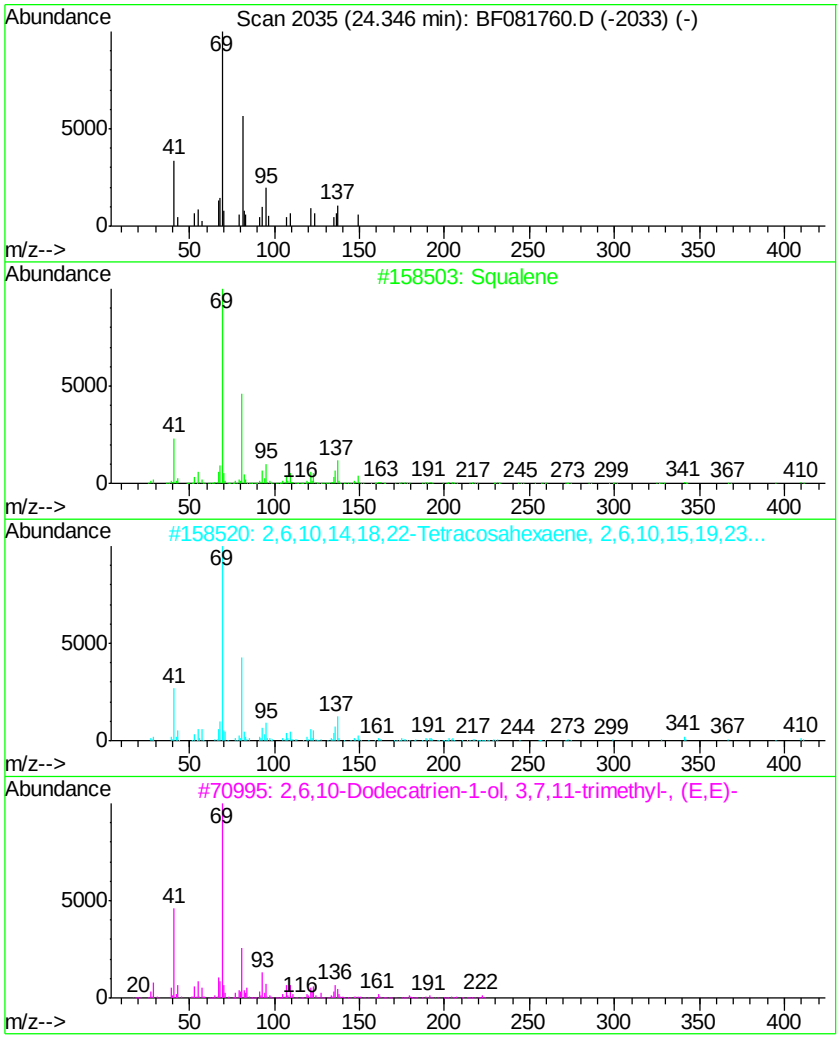
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

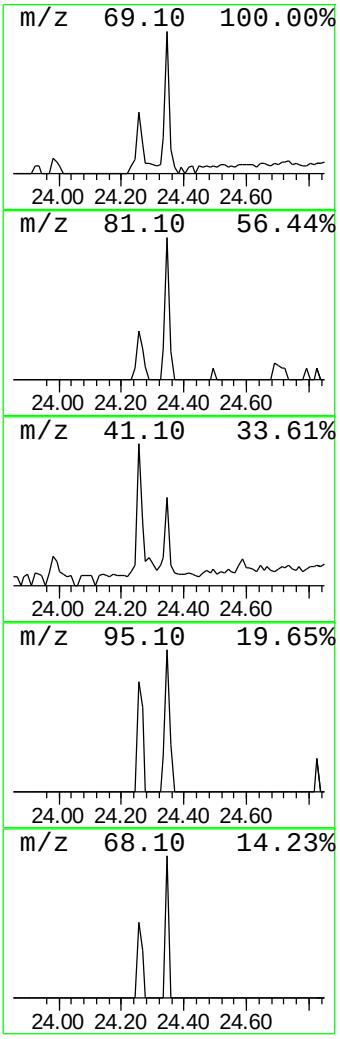
****

Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.35	2.19 ng	22041	Perylene-d12	24.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	86
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	50
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	50
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	50





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Sample : G3748-05
Misc :
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Instrument : BNA_F
ClientSampleId : MGP205-17-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

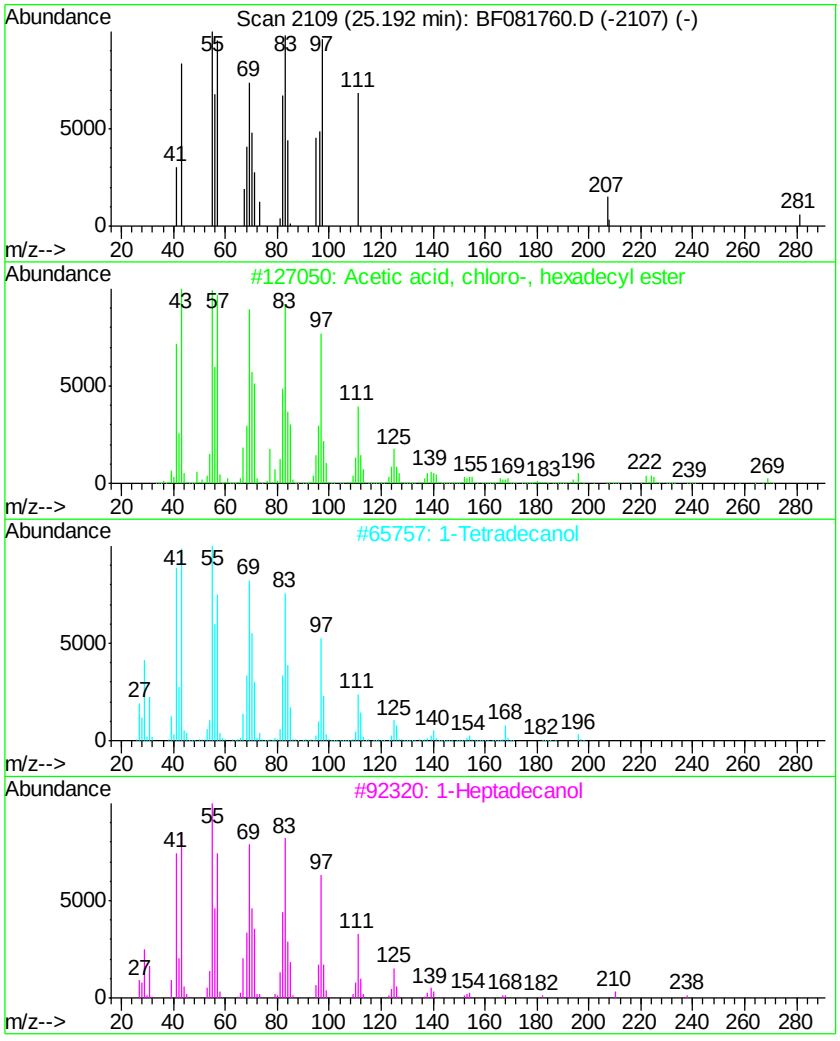
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

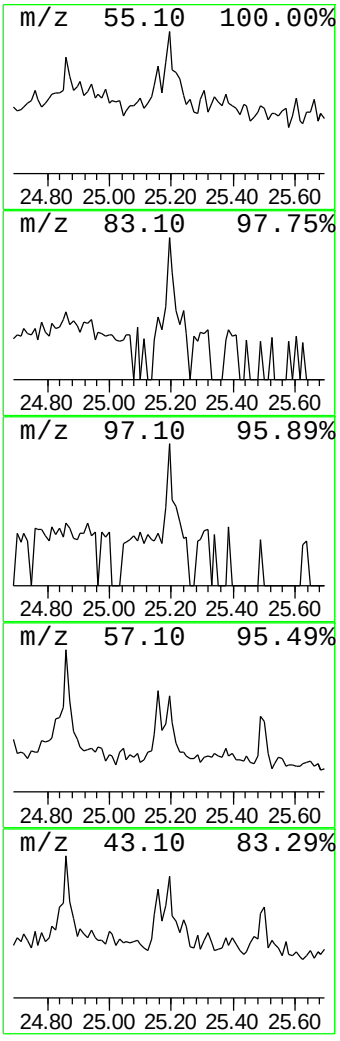
****

Peak Number 10 Acetic acid, chloro-, hexad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.19	2.13 ng	21408	Perylene-d12	24.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	59
2	1-Tetradecanol	214	C14H30O	000112-72-1	53
3	1-Heptadecanol	256	C17H36O	001454-85-9	53
4	1-Hexadecanol	242	C16H34O	036653-82-4	53
5	1-Pentadecanol	228	C15H32O	000629-76-5	53





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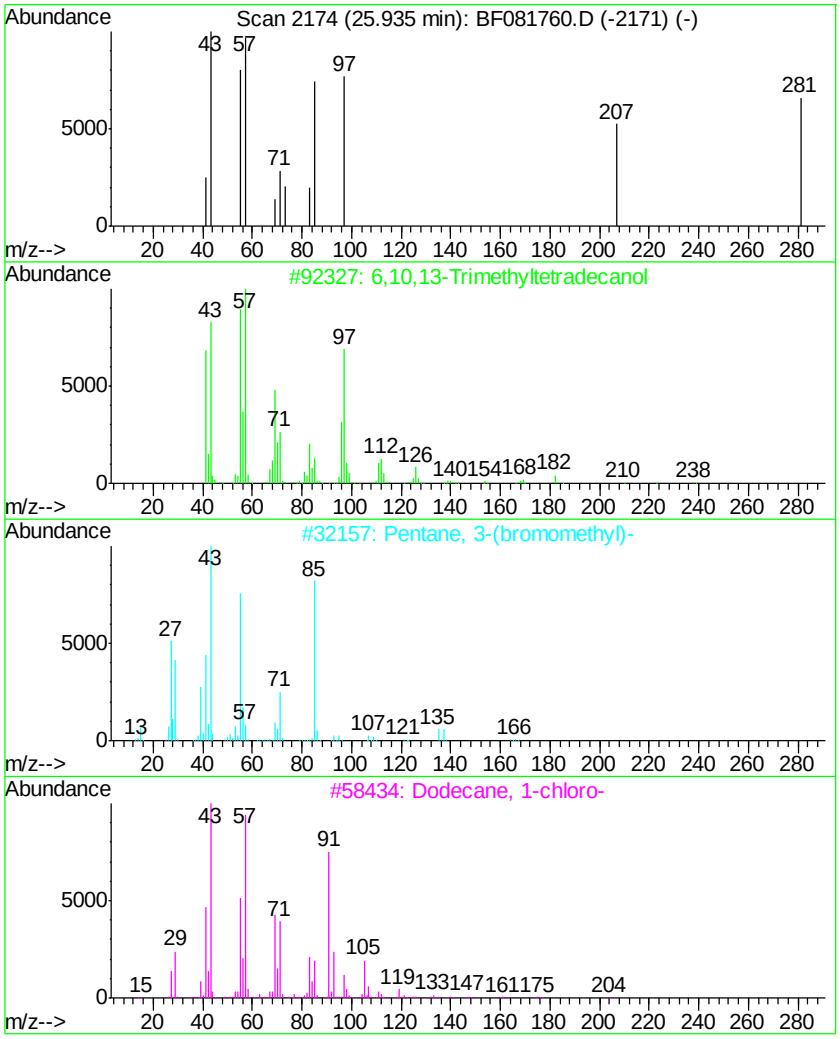
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

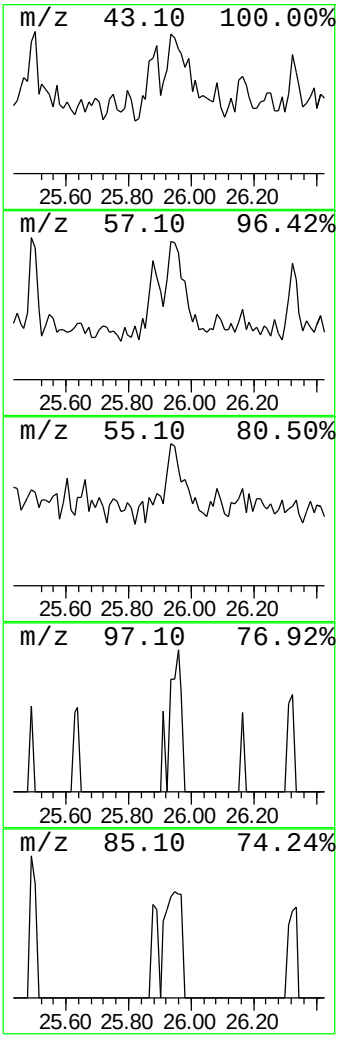
****

Peak Number 11 unknown25.93 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.93	2.27 ng	22848	Perylene-d12	24.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,10,13-Trimethyltetradecanol	256	C17H36O	1000131-71-0	25
2	Pentane, 3-(bromomethyl)-	164	C6H13Br	003814-34-4	10
3	Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	9
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	9
5	3(2H)-Furanone, dihydro-5-isopro...	128	C7H12O2	034004-69-8	9





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	1.26	93.2	ng	1290850	1	8.13	277132	20.0
2-Pentanone, 4-hy...	4.44	67.3	ng	932629	1	8.13	277132	20.0
unknown7.66	7.66	134.8	ng	1868520	1	8.13	277132	20.0
Undecanoic acid	20.43	3.2	ng	62092	4	18.67	384602	20.0
Hexadecanamide	24.25	7.2	ng	72398	6	24.77	201138	20.0
Squalene	24.35	2.2	ng	22041	6	24.77	201138	20.0
Acetic acid, chlo...	25.19	2.1	ng	21408	6	24.77	201138	20.0
unknown25.93	25.93	2.3	ng	22848	6	24.77	201138	20.0