LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103781.D
Acq On : 20 Mar 2018 2:45
Operator : JU/SJ
Sample : J1971-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-2-WW@3

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-BF031518.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	2.328	33	41	47	rVB	153255	211642	4.75%	0.549%
2	5.228	530	534	543	rVB	195852	277367	6.23%	0.720%
3	5.604	592	598	601	rBV	3731178	4307031	96.70%	11.181%
4	5.916	649	651	660	rVB	81415	80408	1.81%	0.209%
5	6.598	760	767	770	rBV	3427267	4454187	100.00%	11.563%
6	6.745	786	792	795	rBV	4038617	4354304	97.76%	11.304%
7	6.969	827	830	834	rVB	1021655	892907	20.05%	2.318%
8	7.128	853	857	861	rBV	3279380	3301479	74.12%	8.571%
9	7.539	921	927	930	rBV	2582742	2836554	63.68%	7.364%
10	8.251	1044	1048	1052	rBV	1387305	1185785	26.62%	3.078%
11	9.327	1226	1231	1234	rBV	4259806	4212783	94.58%	10.936%
12	9.716	1293	1297	1300	rBV	509741	383630	8.61%	0.996%
13	9.927	1329	1333	1336	rBV	104391	79023	1.77%	0.205%
14	10.010	1343	1347	1351	rBV	1314956	1251963	28.11%	3.250%
15	10.427	1415	1418	1421	rVB	129522	96677	2.17%	0.251%
16	10.804	1478	1482	1486	rBV	2428715	2573773	57.78%	6.681%
17	10.904	1496	1499	1505	rVB	101447	103719	2.33%	0.269%
18	11.504	1597	1601	1604	rBV	1317539	1116683	25.07%	2.899%
19	12.016	1684	1688	1693	rBV	98322	101943	2.29%	0.265%
20	13.092	1867	1871	1875	rBV	3208677	3421909	76.82%	8.883%
21	13.974	2017	2021	2030	rBV	646202	627761	14.09%	1.630%
22	14.157	2047	2052	2055	rBV	1051676	941128	21.13%	2.443%
23	14.621	2126	2131	2134	rBV	94777	112387	2.52%	0.292%
24	14.921	2178	2182	2191	rBV	499988	578364	12.98%	1.501%
25	15.698	2308	2314	2325	rBV	579458	803394	18.04%	2.086%
26	16.221	2398	2403	2412	rBV2	77403	145321	3.26%	0.377%
27	17.880	2680	2685	2693	rVB9	30711	69268	1.56%	0.180%

Sum of corrected areas: 38521390

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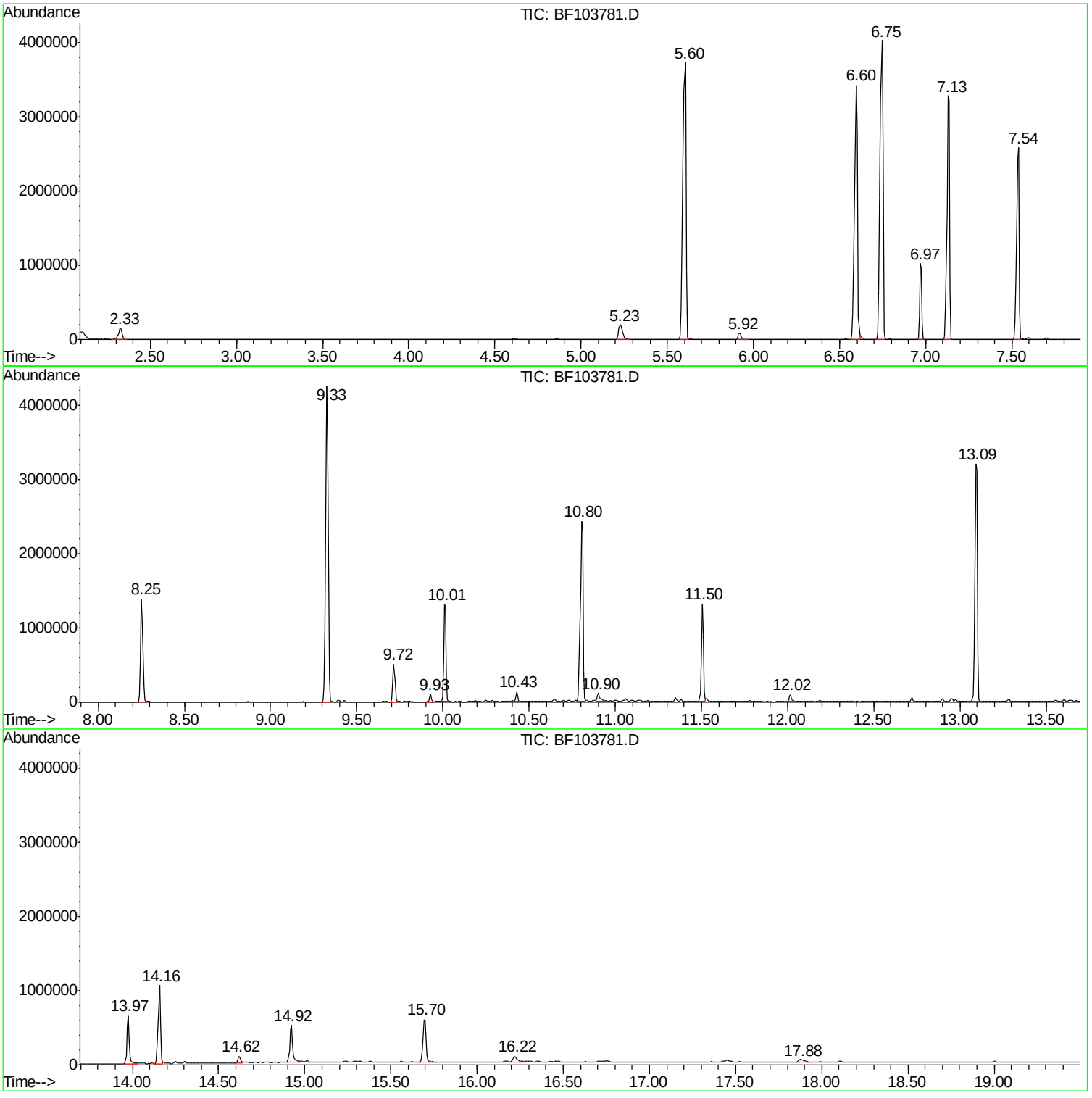
Instrument :
BNA_F
ClientSampleId :
ES-6-SA-2-WW@3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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\BF031918\
Data File : BF103781.D
Acq On : 20 Mar 2018 2:45
Operator : JU/SJ
Sample : J1971-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-2-WW@3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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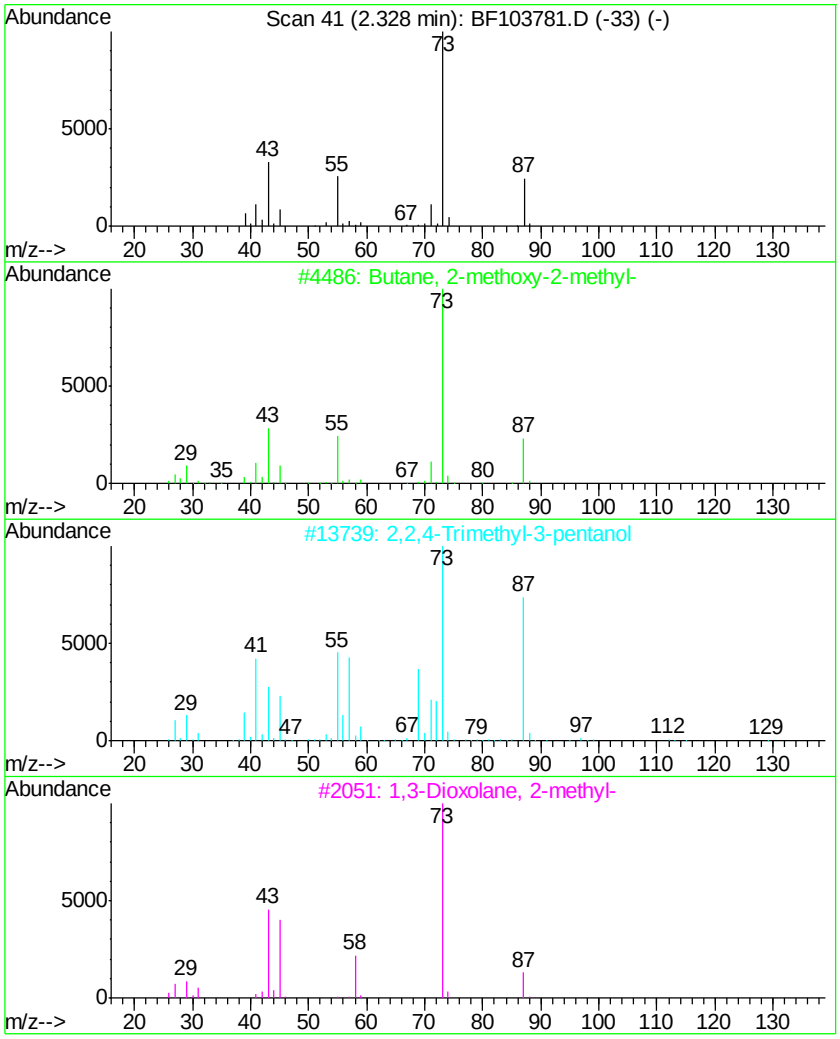
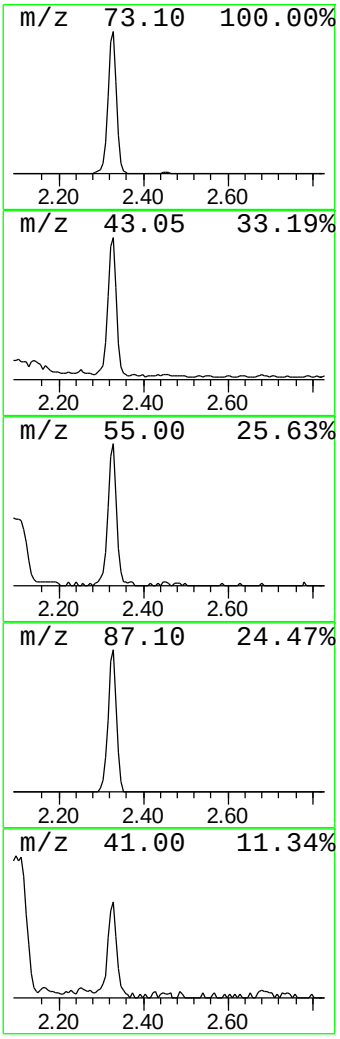
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	4.74 ng	211642	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Sample : J1971-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-2-WW@3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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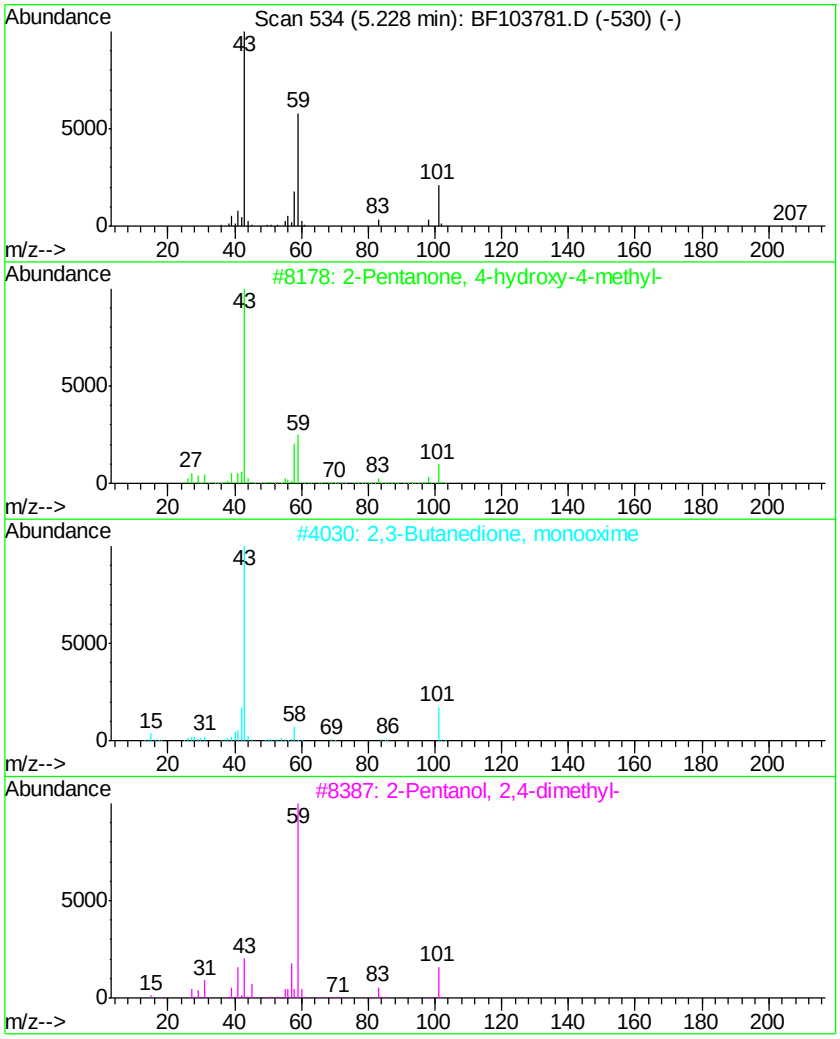
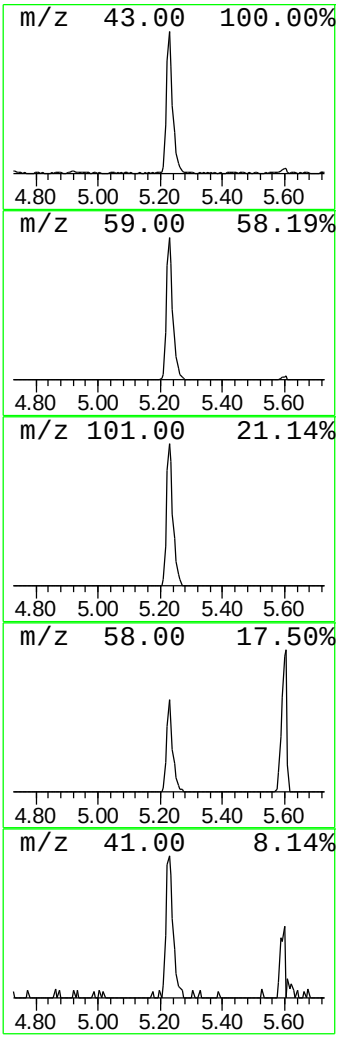
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	6.21 ng	277367	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103781.D
Acq On : 20 Mar 2018 2:45
Operator : JU/SJ
Sample : J1971-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-2-WW@3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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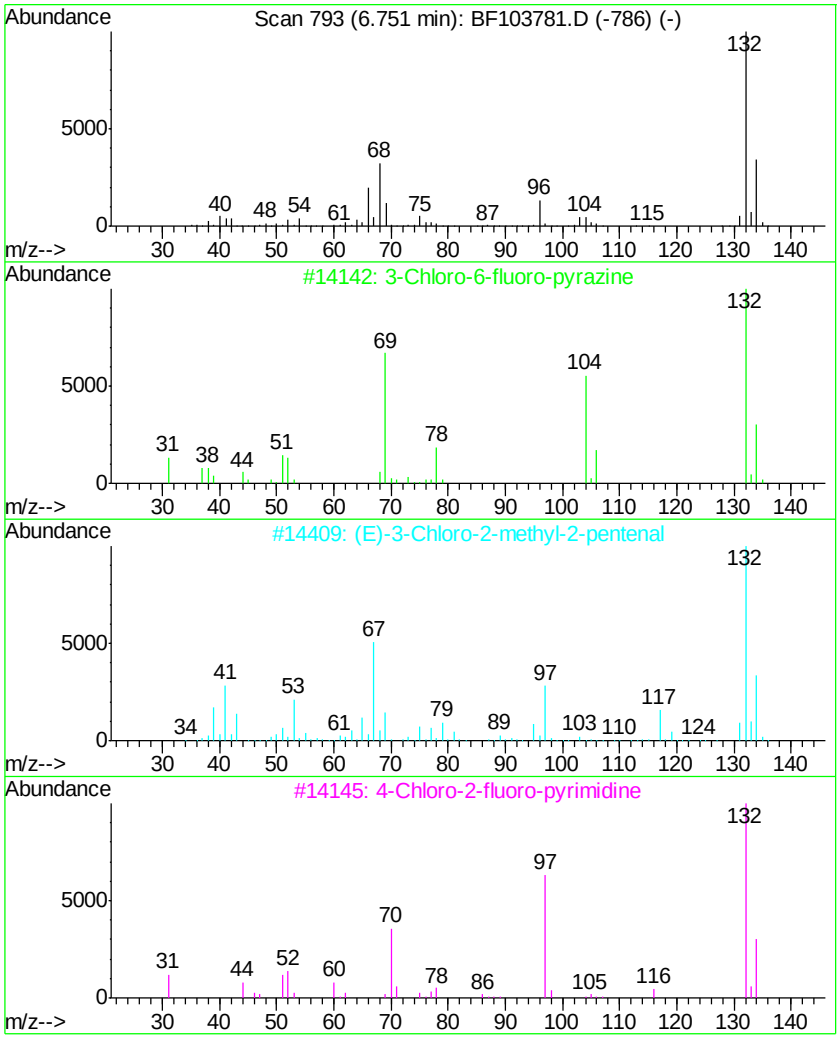
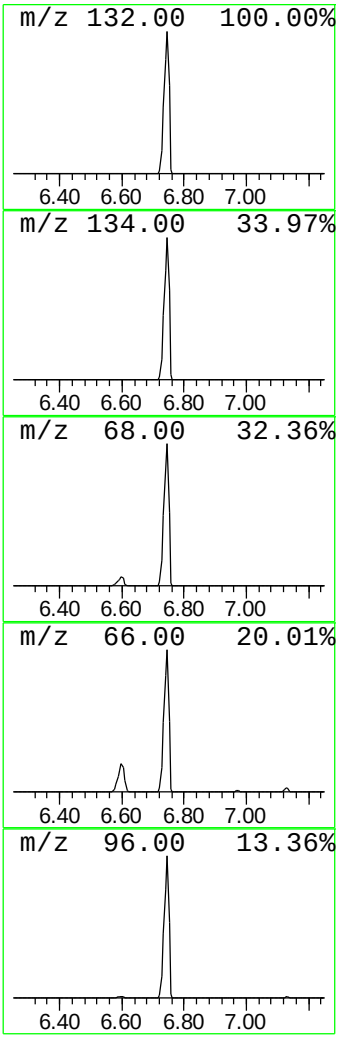
Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	97.53 ng	4354300	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : J1971-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-2-WW@3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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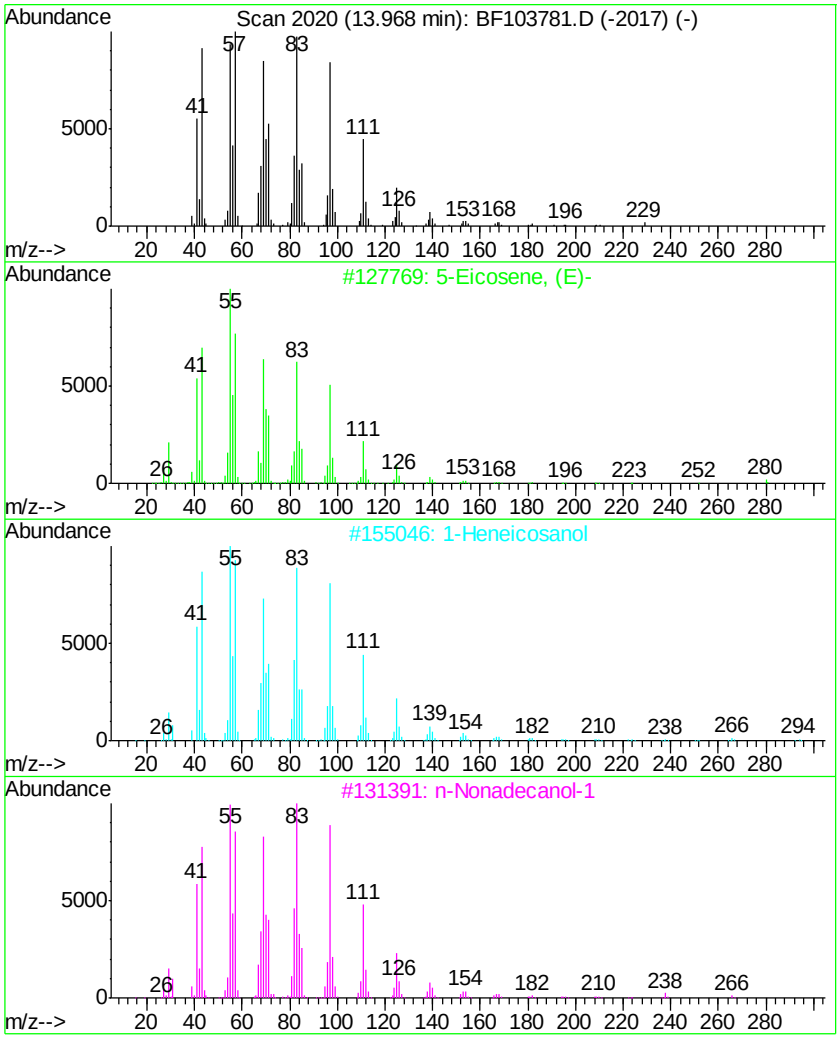
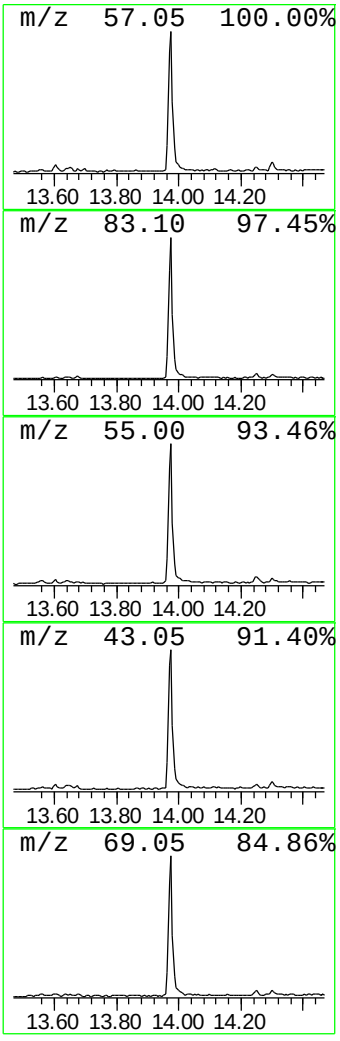
Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	13.34 ng	627761	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93





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Operator : JU/SJ
Sample : J1971-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-2-WW@3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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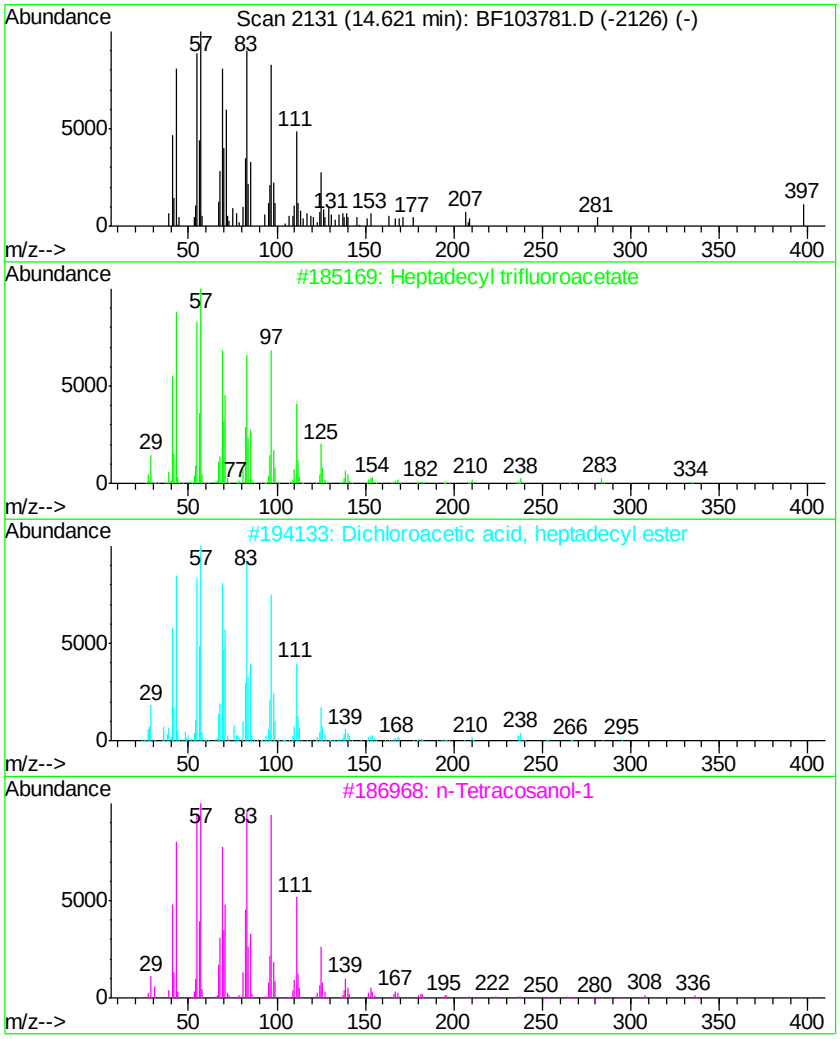
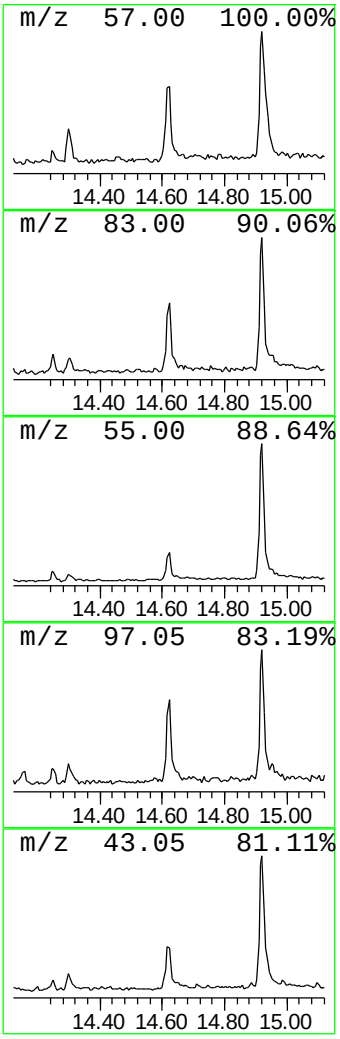
Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.39 ng	112387	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90





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Misc :
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Instrument : BNA_F
ClientSampleId : ES-6-SA-2-WW@3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

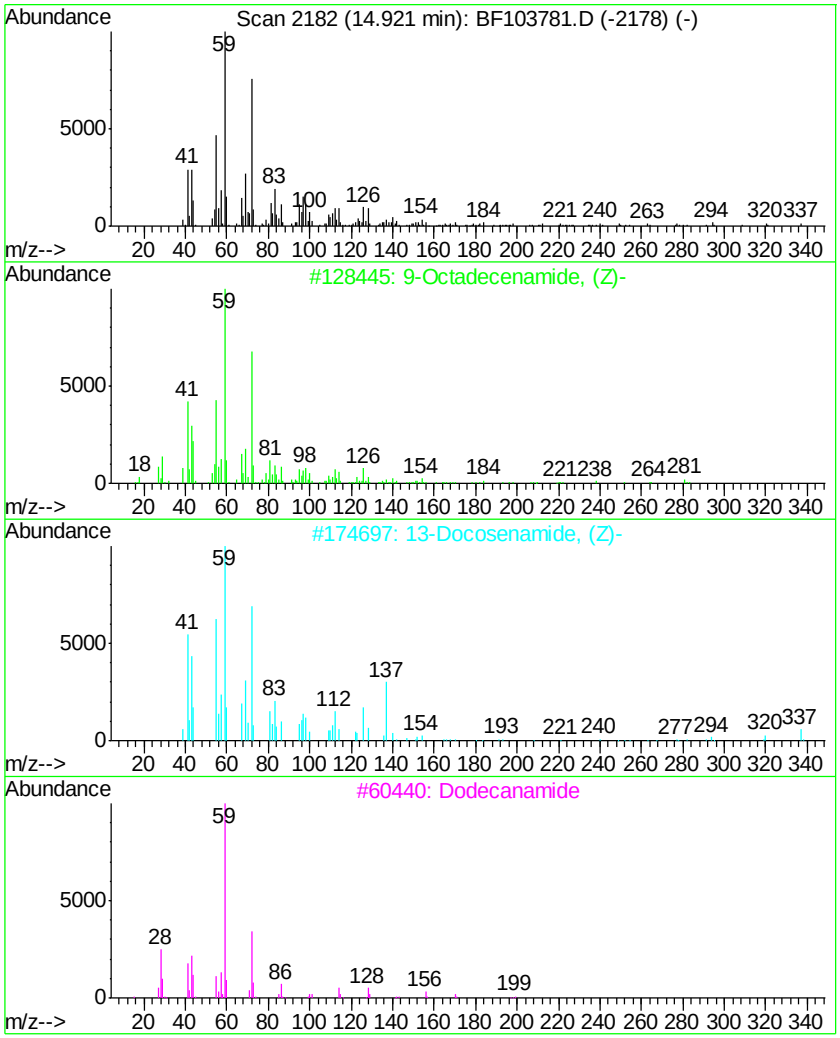
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

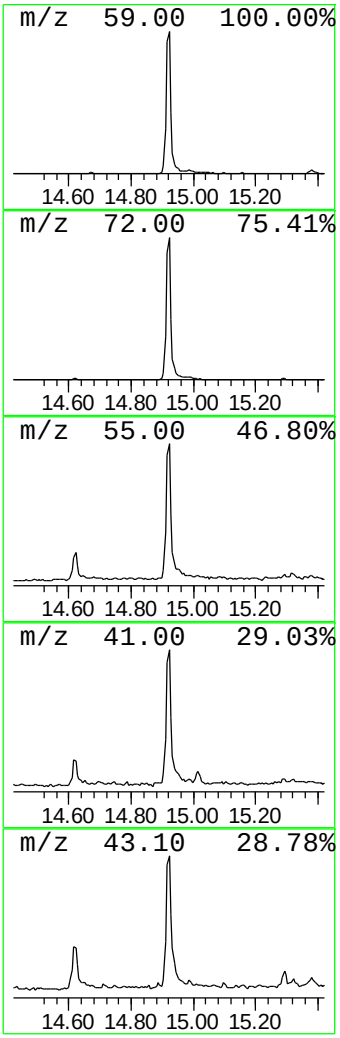
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	12.29 ng	578364	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	78
3	Dodecanamide	199	C12H25NO	001120-16-7	38
4	1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	38
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	38





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Instrument : BNA_F
ClientSampleId : ES-6-SA-2-WW@3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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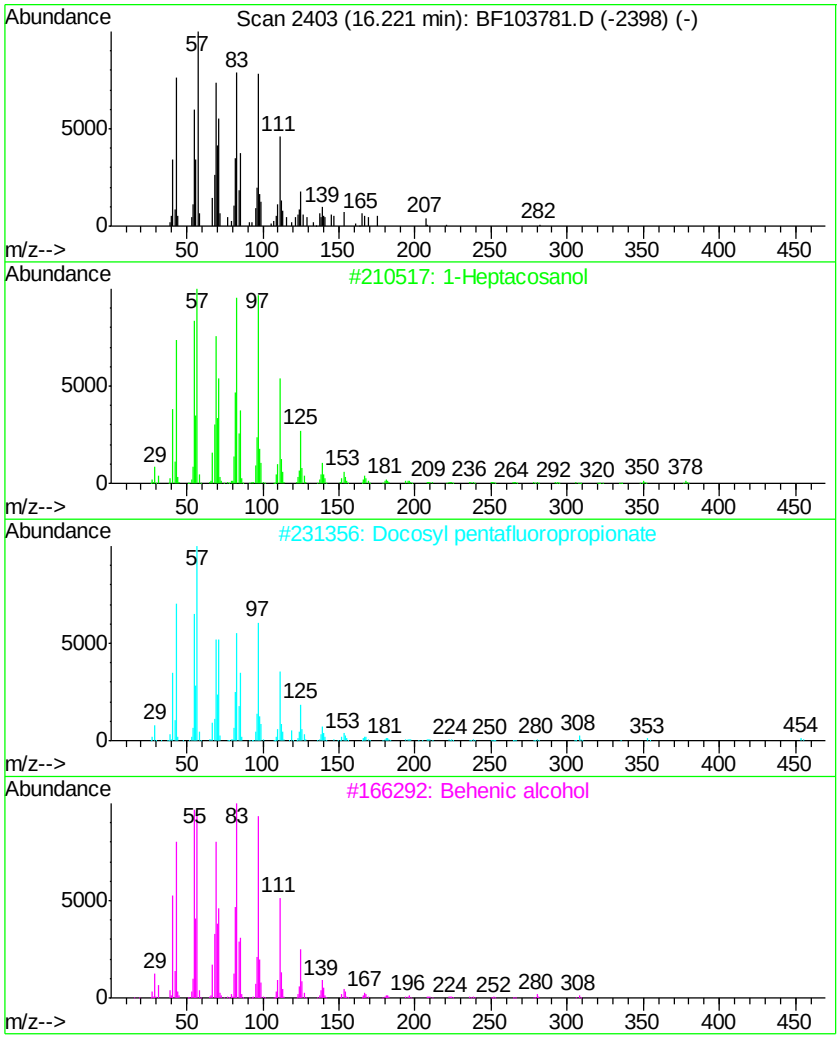
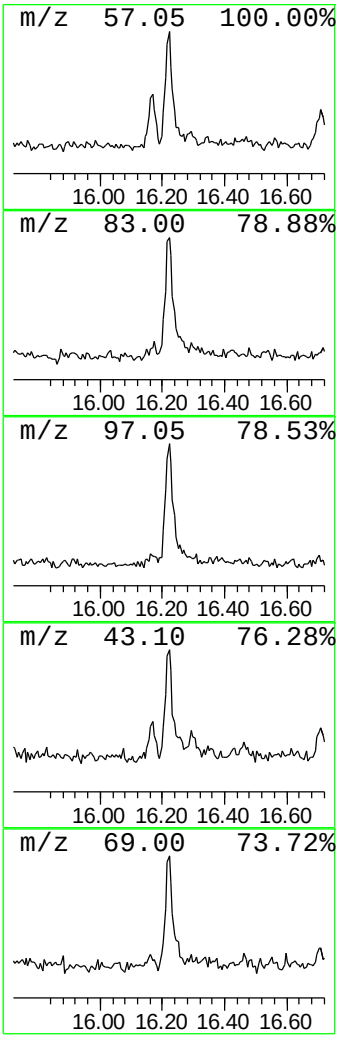
Peak Number 8 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	3.62 ng	145321	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	89
3	Behenic alcohol	326	C22H46O	000661-19-8	87
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	86
5	Octacosanol	410	C28H58O	000557-61-9	86





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	2.33	4.7	ng	211642	1	6.97	892907	20.0
2-Pentanone, 4-hy...	5.23	6.2	ng	277367	1	6.97	892907	20.0
unknown6.75	6.75	97.5	ng	4354300	1	6.97	892907	20.0
5-Eicosene, (E)-	13.97	13.3	ng	627761	5	14.16	941128	20.0
Heptadecyl triflu...	14.62	2.4	ng	112387	5	14.16	941128	20.0
9-Octadecenamide,...	14.92	12.3	ng	578364	5	14.16	941128	20.0
1-Heptacosanol	16.22	3.6	ng	145321	6	15.70	803394	20.0