LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103777.D
Acq On : 20 Mar 2018 00:58
Operator : JU/SJ
Sample : J1971-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-1-WW@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-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	35	41	46	rVB	154649	208924	5.25%	0.600%
2	5.228	529	534	542	rVB	150678	209406	5.27%	0.602%
3	5.604	592	598	601	rBV	3355101	3931517	98.87%	11.300%
4	5.922	648	652	658	rVB	47750	48339	1.22%	0.139%
5	6.598	760	767	770	rBV	3345053	3976377	100.00%	11.429%
6	6.745	787	792	795	rBV	3854594	3935481	98.97%	11.311%
7	6.969	827	830	834	rBV	961691	846356	21.28%	2.433%
8	7.128	853	857	861	rBV	3100160	3002060	75.50%	8.629%
9	7.534	921	926	929	rBV	2304226	2530154	63.63%	7.272%
10	7.592	932	936	941	rVB	35851	40908	1.03%	0.118%
11	8.251	1044	1048	1052	rBV	1286482	1109205	27.89%	3.188%
12	9.328	1226	1231	1234	rBV	4003011	3878585	97.54%	11.148%
13	9.716	1293	1297	1300	rBV	343191	263582	6.63%	0.758%
14	9.928	1329	1333	1336	rBV	125100	90292	2.27%	0.260%
15	10.010	1343	1347	1351	rBV	1228241	1150785	28.94%	3.308%
16	10.428	1416	1418	1421	rVB	152866	108006	2.72%	0.310%
17	10.645	1449	1455	1458	rBV	35608	47834	1.20%	0.137%
18	10.804	1478	1482	1486	rBV	2354843	2307352	58.03%	6.632%
19	10.904	1495	1499	1508	rVB	107381	132180	3.32%	0.380%
20	11.351	1572	1575	1577	rBV	69653	50522	1.27%	0.145%
21	11.504	1597	1601	1604	rBV	1197413	1041306	26.19%	2.993%
22	12.016	1684	1688	1693	rBV	100644	93067	2.34%	0.267%
23	13.098	1867	1872	1875	rBV	3016425	3141223	79.00%	9.029%
24	13.974	2017	2021	2030	rBV	551278	529483	13.32%	1.522%
25	14.157	2048	2052	2055	rBV	991390	874516	21.99%	2.514%
26	14.621	2127	2131	2137	rBV2	49861	64758	1.63%	0.186%
27	14.915	2178	2181	2192	rBV	238458	293649	7.38%	0.844%
28	15.698	2308	2314	2319	rBV	582966	776556	19.53%	2.232%
29	16.221	2399	2403	2411	rVB2	63716	109826	2.76%	0.316%

Sum of corrected areas: 34792249

LSC Report - Integrated Chromatogram

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Operator : JU/SJ
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Misc :
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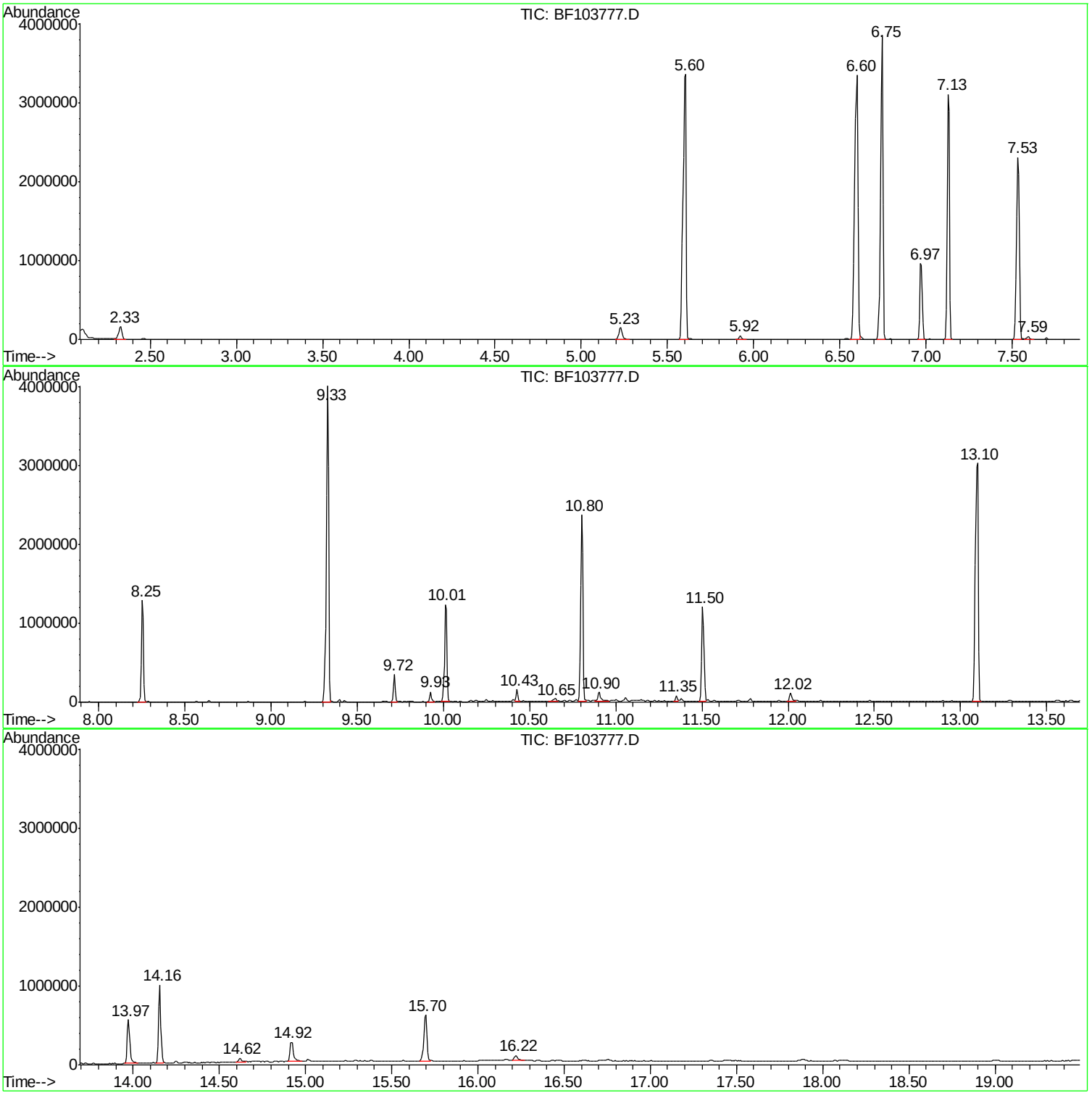
Instrument : BNA_F
ClientSampleId : ES-6-SA-1-WW@2

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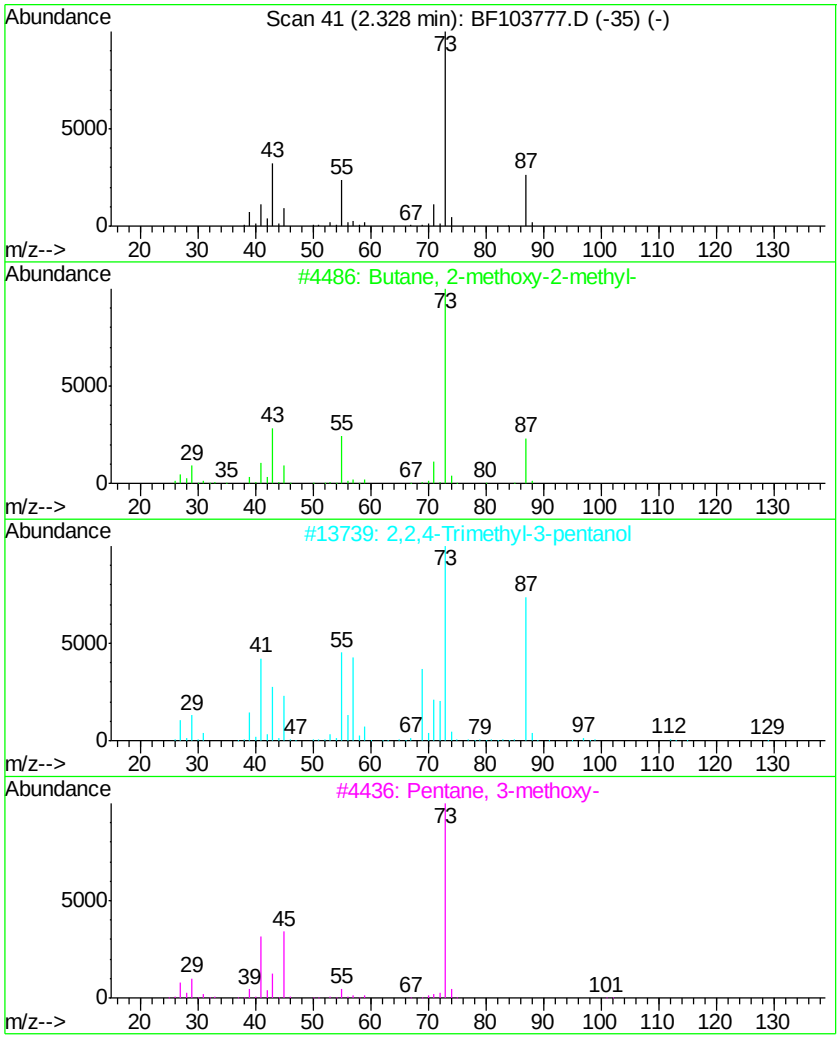
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

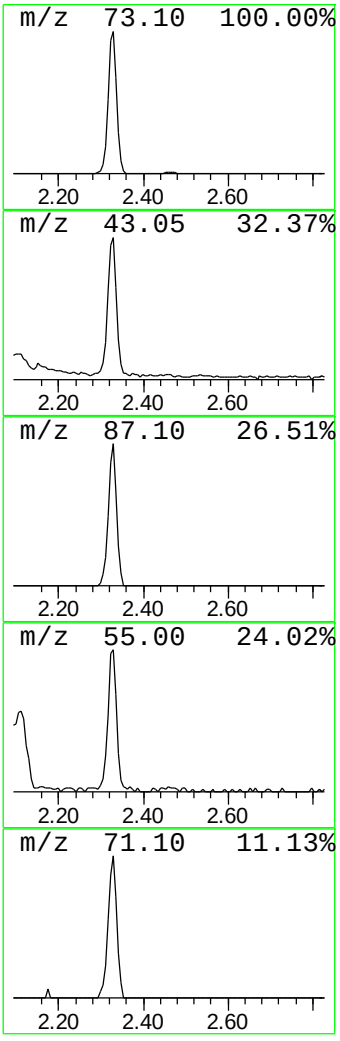
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	4.94 ng	208924	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	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
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Acq On : 20 Mar 2018 00:58
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Sample : J1971-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-1-WW@2

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

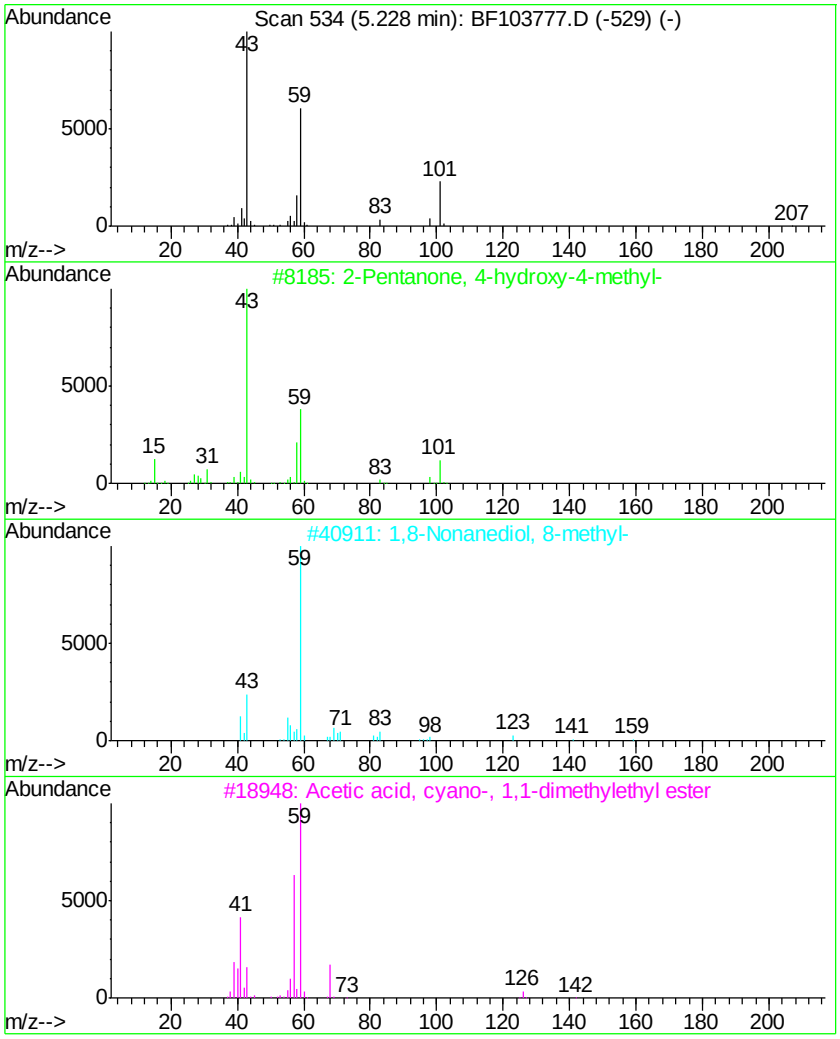
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

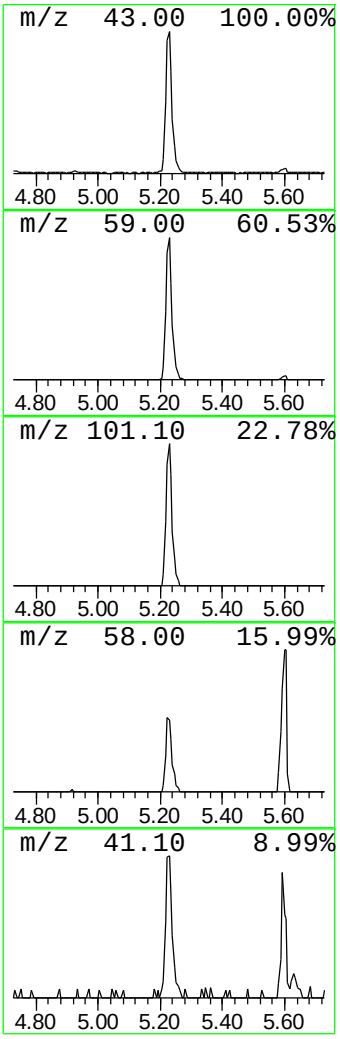
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	4.95 ng	209406	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	56
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Sample : J1971-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-1-WW@2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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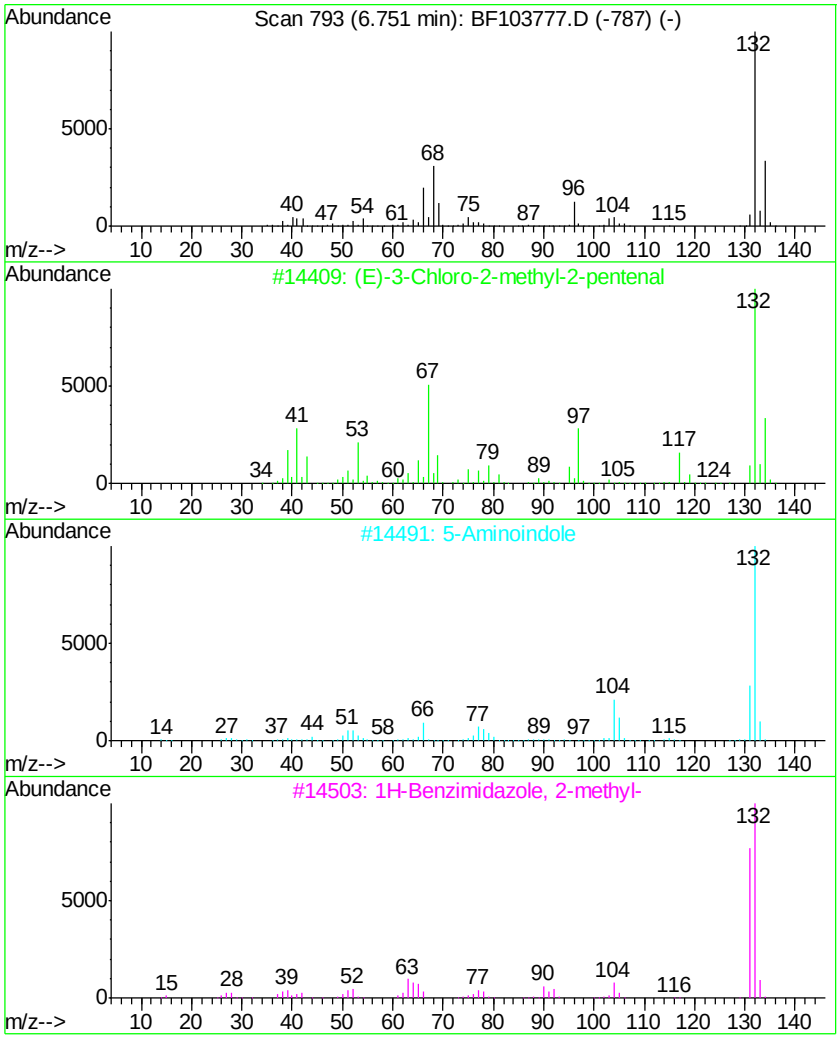
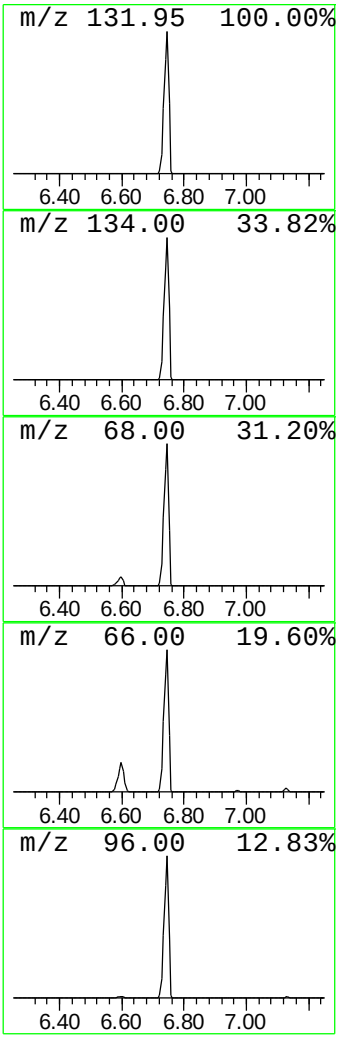
Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	93.00 ng	3935480	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Operator : JU/SJ
Sample : J1971-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ES-6-SA-1-WW@2

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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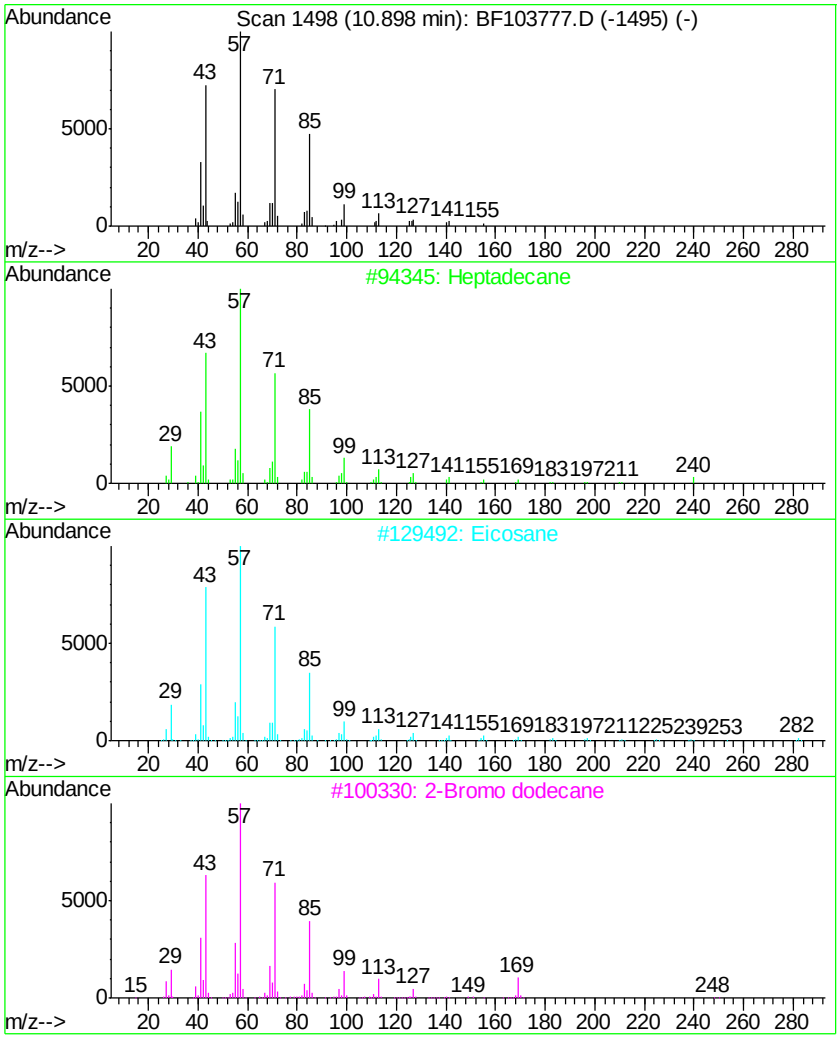
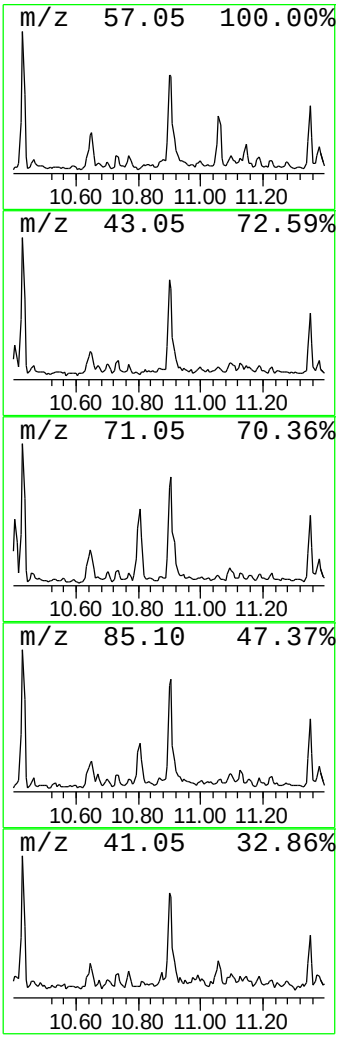
Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.54 ng	132180	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Eicosane	282	C20H42	000112-95-8	90
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
4	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	90
5	Hexadecane	226	C16H34	000544-76-3	90





Library Search Compound Report

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

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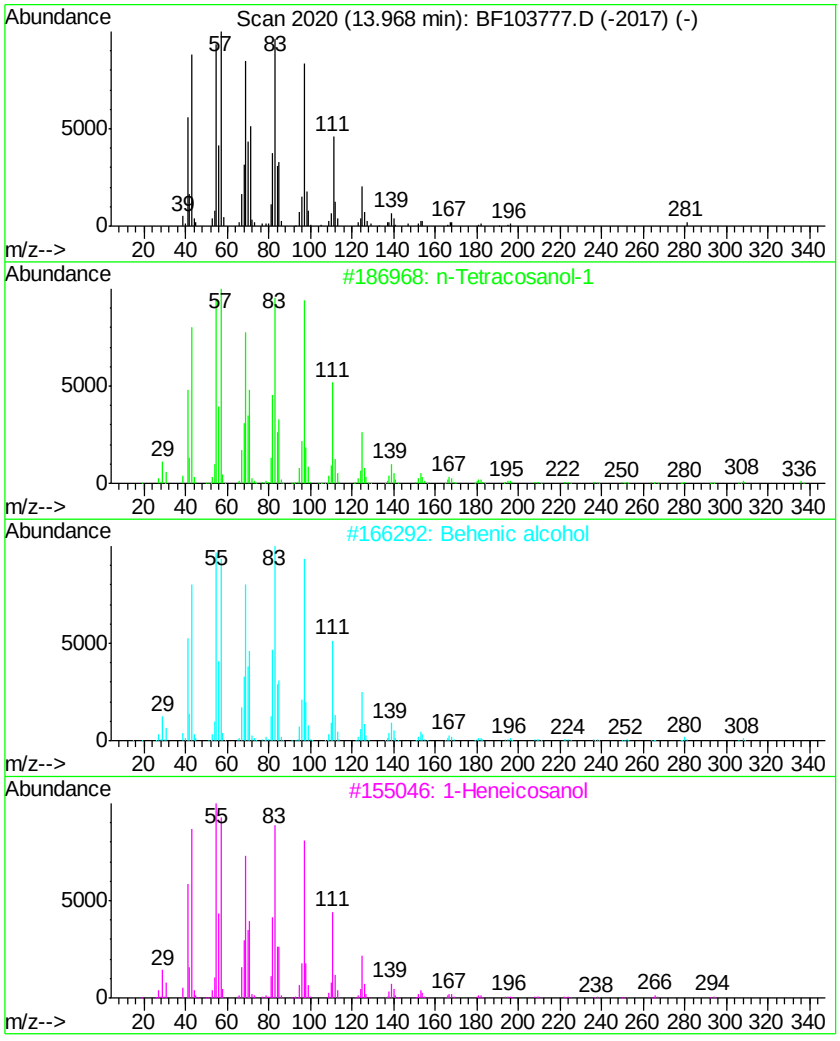
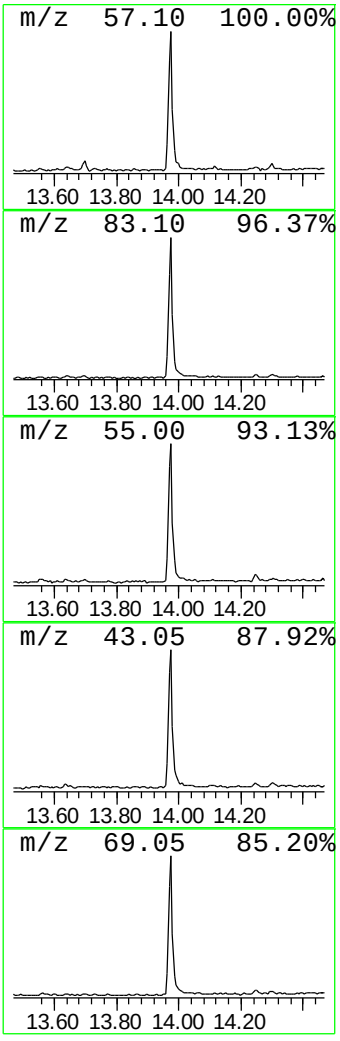
Peak Number 6 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	12.11 ng	529483	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





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Instrument : BNA_F
ClientSampleId : ES-6-SA-1-WW@2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
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TIC Library : C:\DATABASE\NIST11.L
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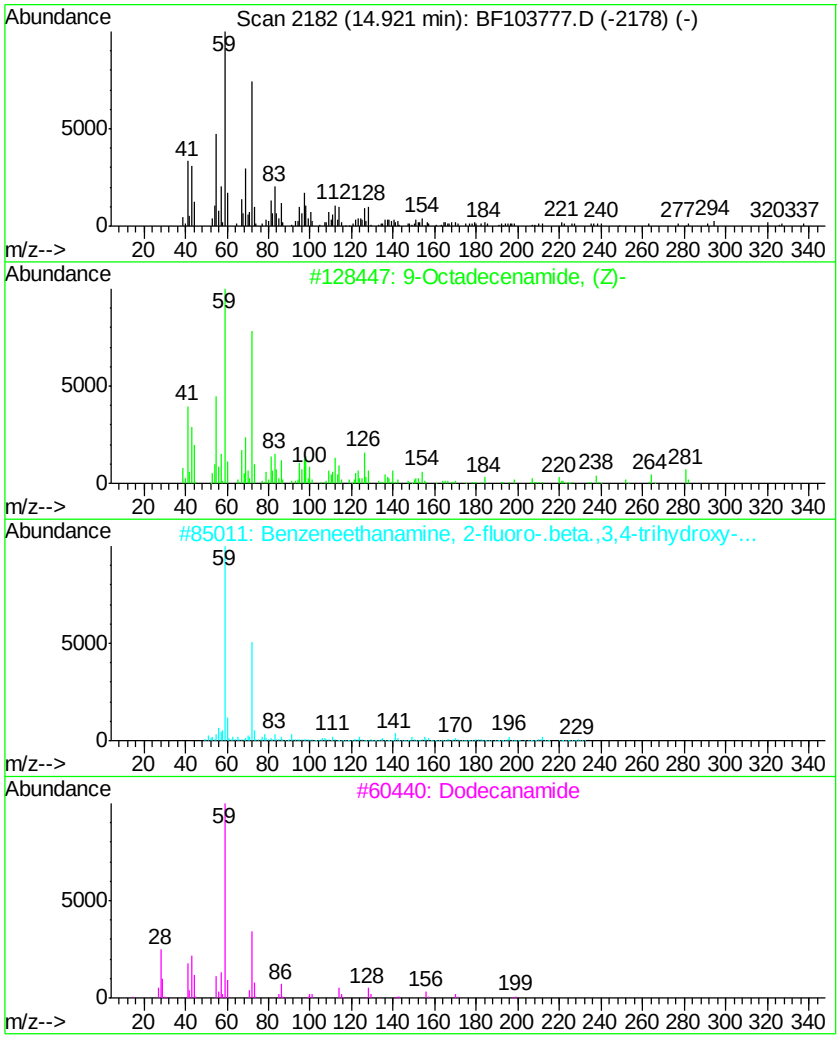
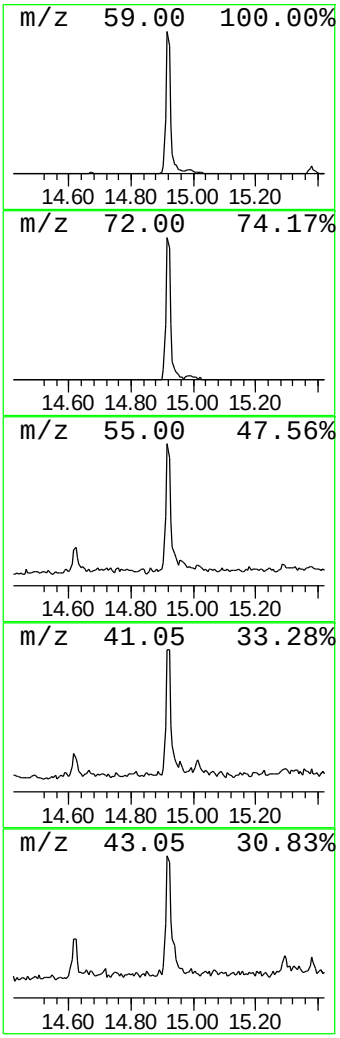
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	6.72 ng	293649	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	47
3	Dodecanamide	199	C12H25NO	001120-16-7	43
4	2-Methyl-2-decanol	172	C11H24O	003396-02-9	43
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	43





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

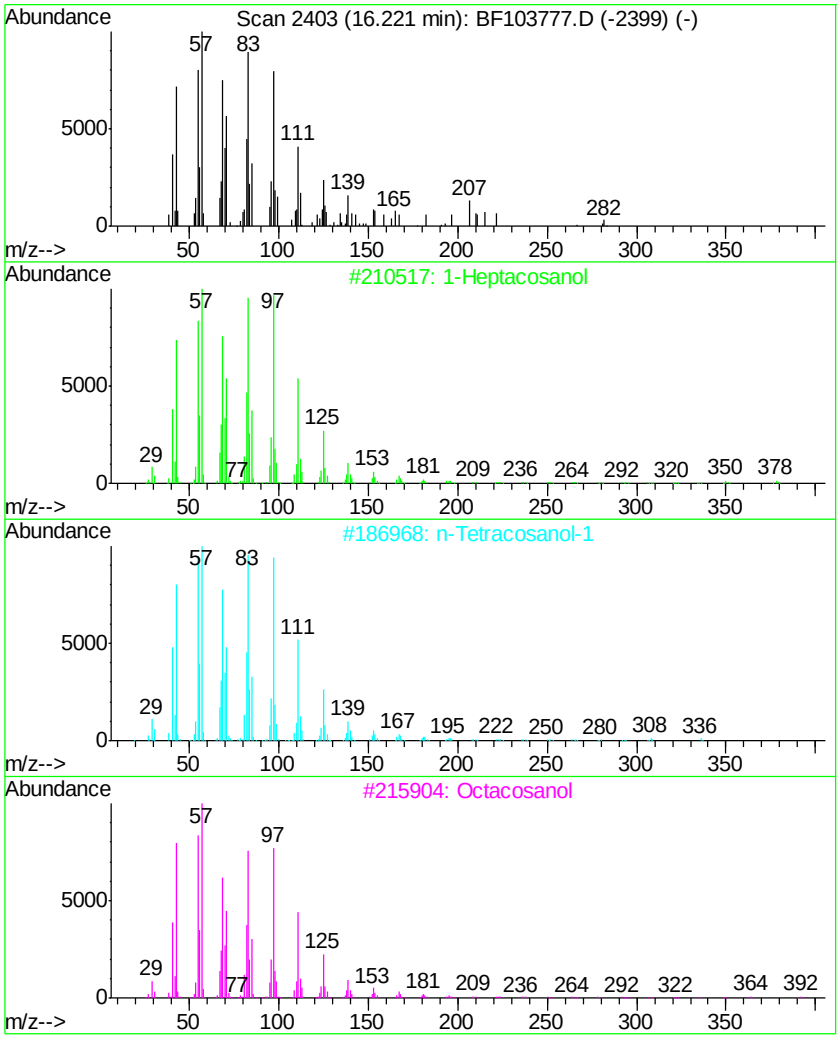
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

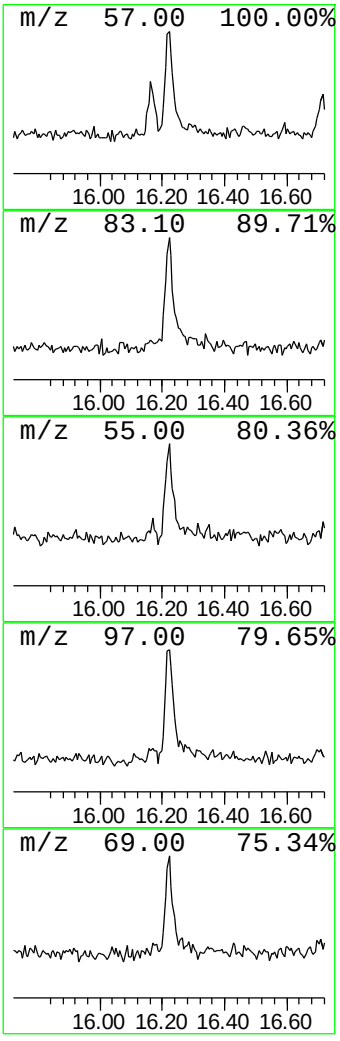
****

Peak Number 8 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.83 ng	109826	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Octacosanol	410	C28H58O	000557-61-9	93
4	Cyclopentadecane	210	C15H30	000295-48-7	92
5	Behenic alcohol	326	C22H46O	000661-19-8	90





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.33	4.9	ng	208924	1	6.97	846356	20.0
2-Pentanone, 4-hy...	5.23	5.0	ng	209406	1	6.97	846356	20.0
unknown6.75	6.75	93.0	ng	3935480	1	6.97	846356	20.0
Heptadecane	10.90	2.5	ng	132180	4	11.50	1041310	20.0
n-Tetracosanol-1	13.97	12.1	ng	529483	5	14.16	874516	20.0
9-Octadecenamide,...	14.92	6.7	ng	293649	5	14.16	874516	20.0
1-Heptacosanol	16.22	2.8	ng	109826	6	15.70	776556	20.0