LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110569.D
Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-J

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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	2.257	24	29	40	rVB	214036	313871	25.53%	2.622%
2	5.187	523	527	536	rBV	33662	47929	3.90%	0.400%
3	5.575	589	593	612	rBV	1178321	1184192	96.34%	9.891%
4	6.575	759	763	780	rBV	1250746	1229199	100.00%	10.267%
5	6.722	784	788	791	rBV	1435300	1216618	98.98%	10.162%
6	6.951	824	827	834	rBV	453739	379331	30.86%	3.168%
7	7.104	850	853	868	rVB	1000252	941782	76.62%	7.866%
8	7.516	919	923	937	rBV	683170	713393	58.04%	5.959%
9	8.234	1041	1045	1064	rBV	382573	426435	34.69%	3.562%
10	9.304	1224	1227	1237	rBV	1108242	1076422	87.57%	8.991%
11	9.698	1291	1294	1300	rBV	100405	104573	8.51%	0.873%
12	9.992	1341	1344	1352	rBV	400929	383477	31.20%	3.203%
13	10.786	1475	1479	1490	rBV	614949	567797	46.19%	4.742%
14	11.486	1595	1598	1601	rBV	365652	361368	29.40%	3.018%
15	11.510	1601	1602	1608	rVB	68801	60029	4.88%	0.501%
16	11.992	1681	1684	1688	rBV	69419	71040	5.78%	0.593%
17	12.704	1802	1805	1811	rBV	151298	143504	11.67%	1.199%
18	12.774	1815	1817	1821	rBV5	15569	20667	1.68%	0.173%
19	12.939	1842	1845	1850	rVB	127305	116207	9.45%	0.971%
20	13.069	1863	1867	1871	rBV	1141548	997544	81.15%	8.332%
21	13.263	1896	1900	1906	rBV6	14319	24533	2.00%	0.205%
22	13.498	1937	1940	1943	rBV5	21739	28479	2.32%	0.238%
23	13.616	1957	1960	1963	rBV5	14562	17502	1.42%	0.146%
24	13.945	2013	2016	2021	rBV3	105366	126882	10.32%	1.060%
25	14.139	2044	2049	2052	rBV	525940	556895	45.31%	4.651%
26	14.163	2052	2053	2059	rVB	88537	79820	6.49%	0.667%
27	14.886	2174	2176	2179	rVB	52581	48096	3.91%	0.402%
28	15.039	2199	2202	2206	rVB	82480	95598	7.78%	0.798%
29	15.239	2233	2236	2239	rVB	95353	105021	8.54%	0.877%
30	15.268	2239	2241	2246	rVB5	40432	60123	4.89%	0.502%
31	15.639	2301	2304	2305	rBV	51399	54629	4.44%	0.456%
32	15.668	2306	2309	2315	rVB	211185	265100	21.57%	2.214%
33	16.092	2377	2381	2387	rVB	96124	154553	12.57%	1.291%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110569.D
Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-J

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

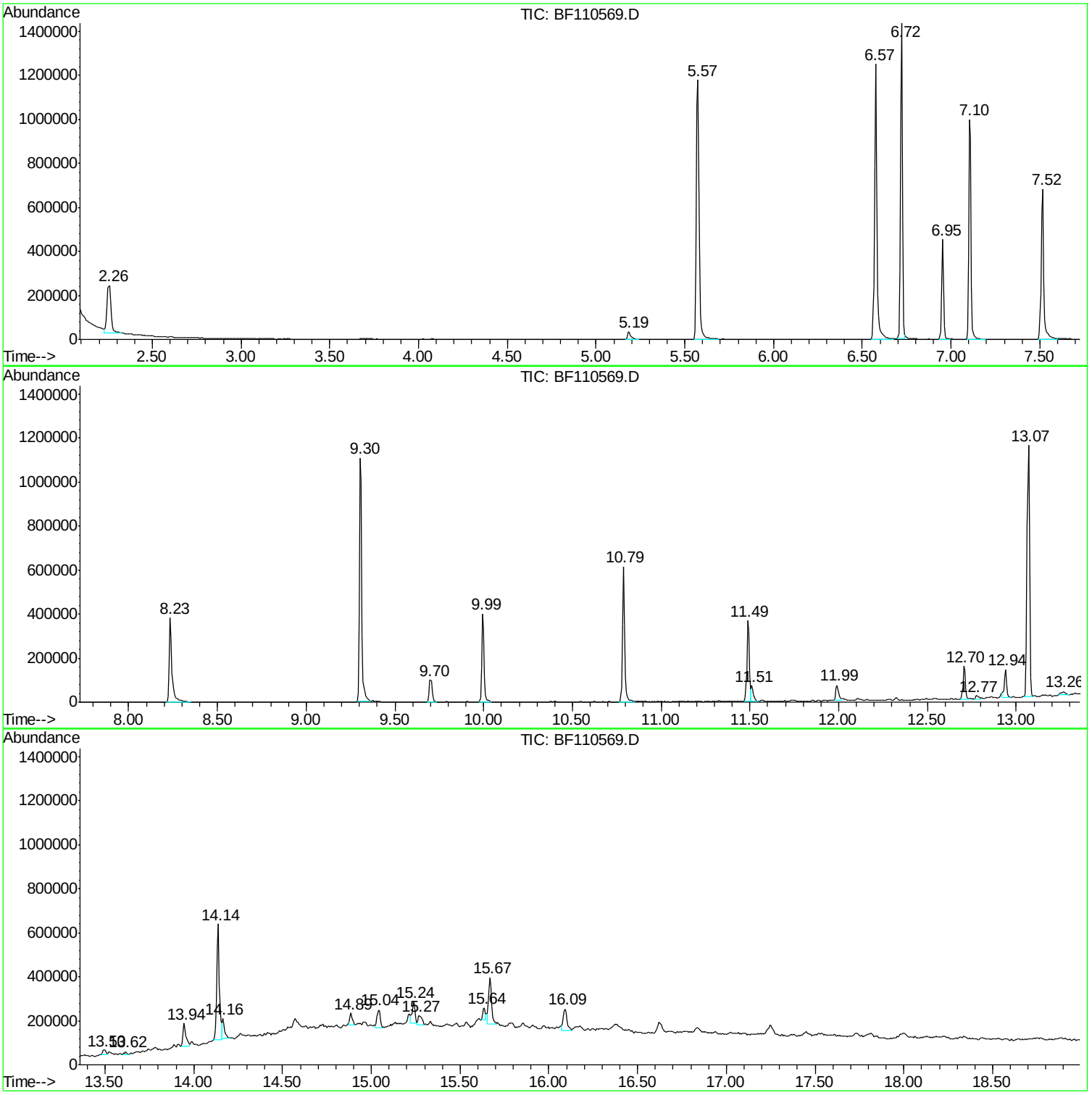
Sum of corrected areas: 11972609

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110569.D
Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110569.D
Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

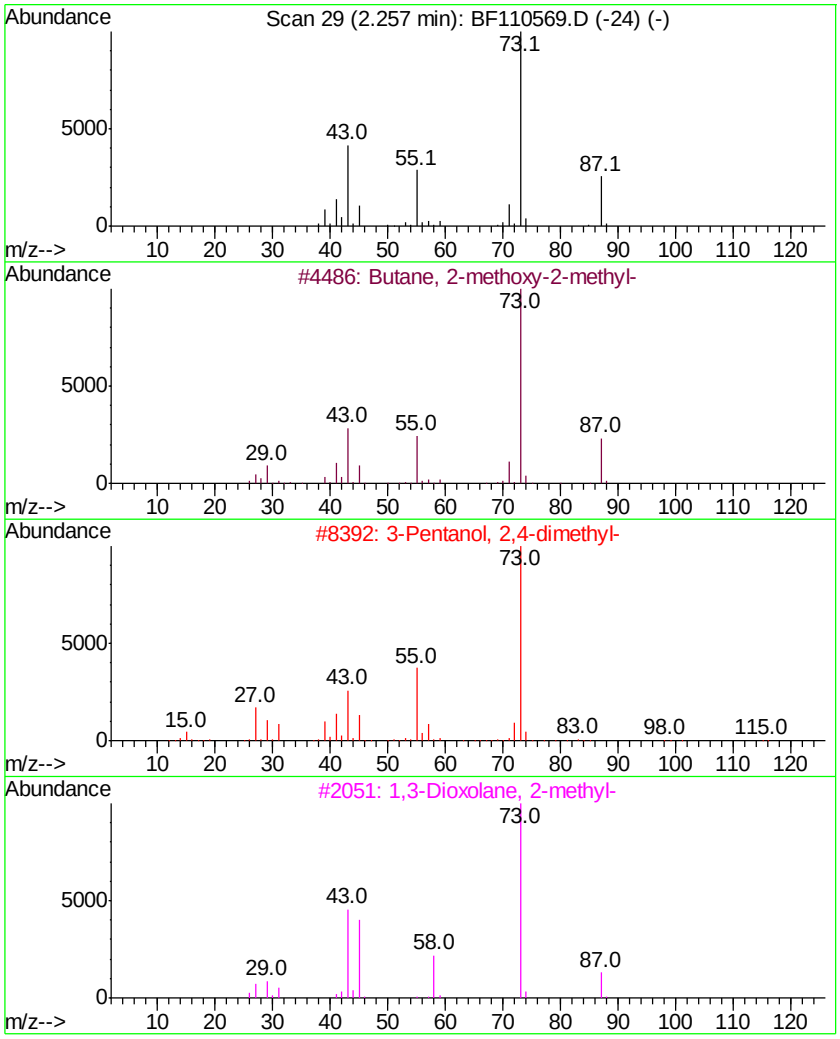
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

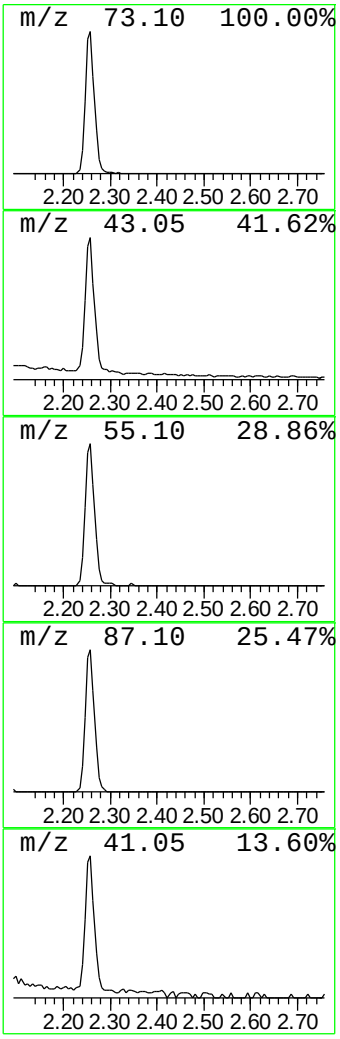
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	16.55 ng	313871	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

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Data File : BF110569.D
Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

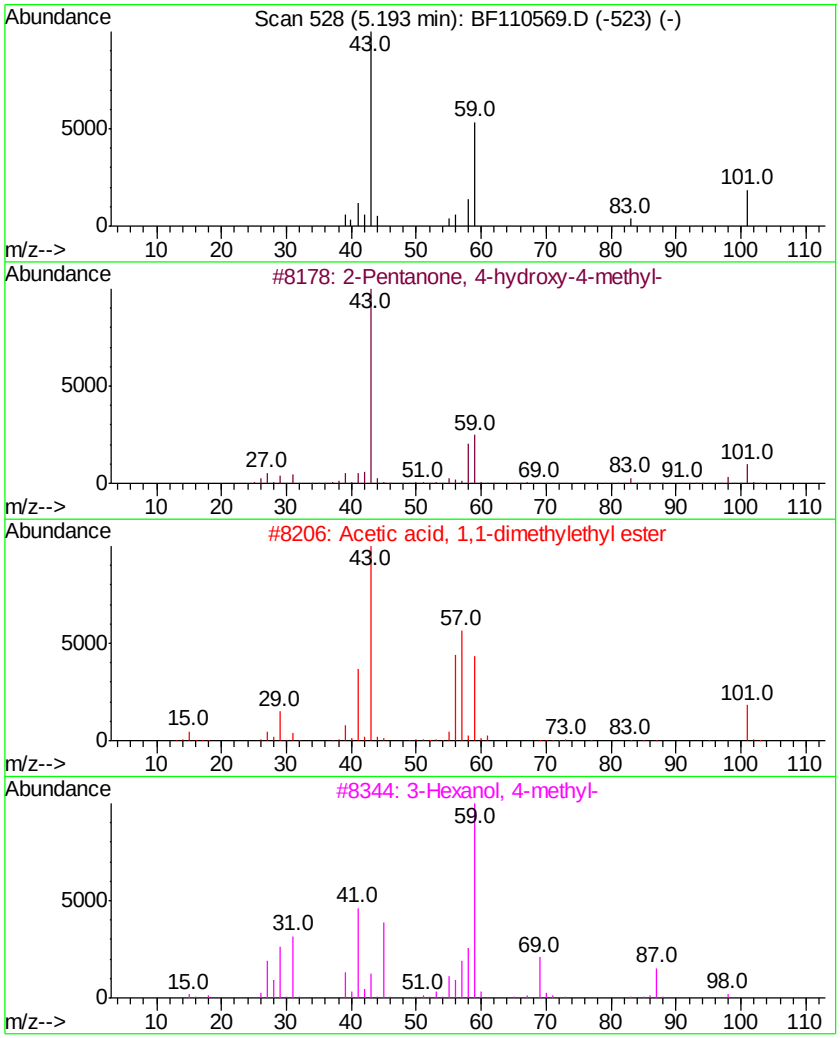
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

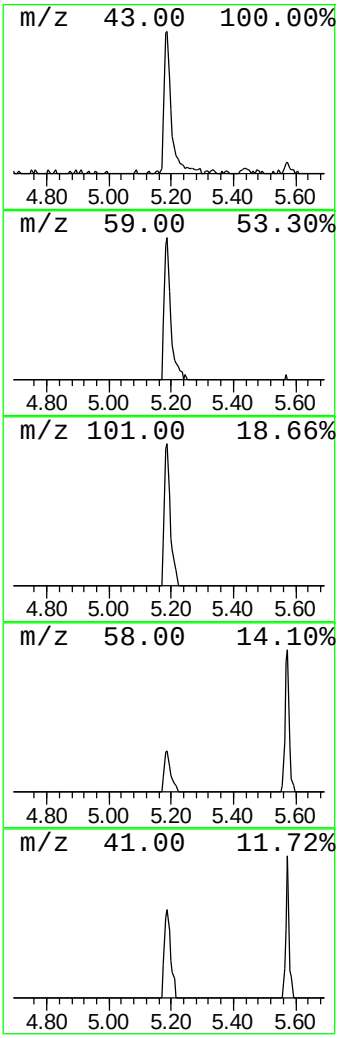
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.53 ng	47929	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
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Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

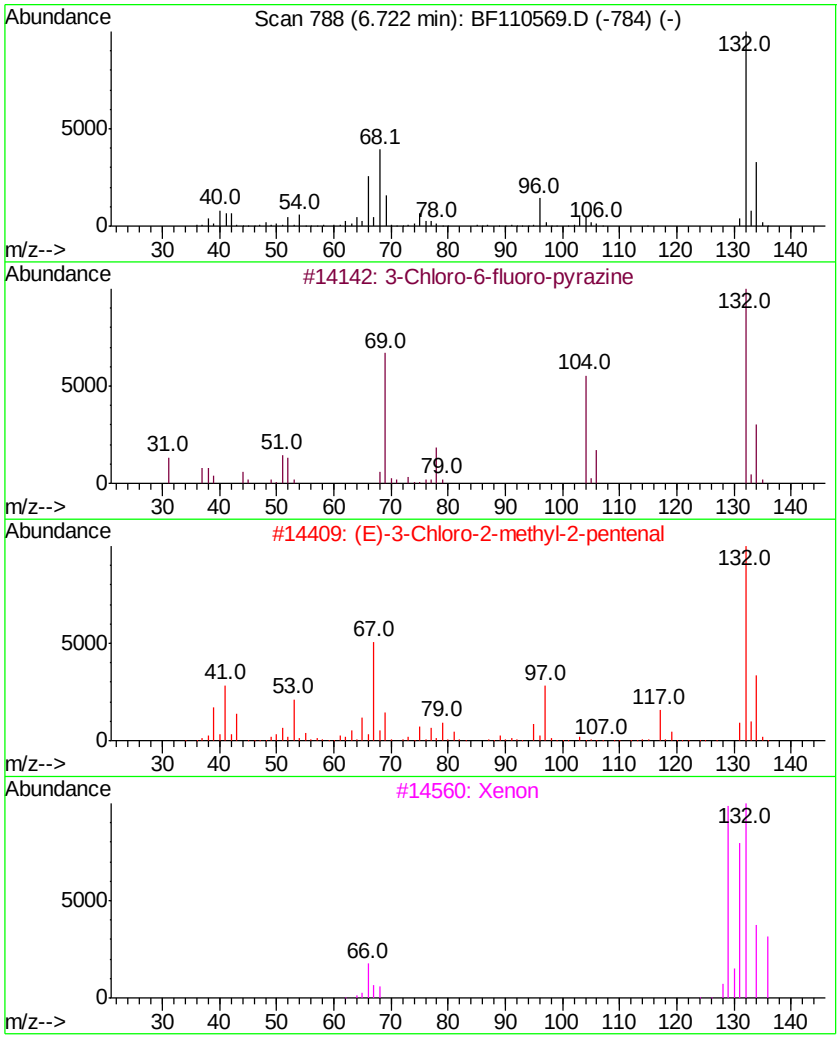
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

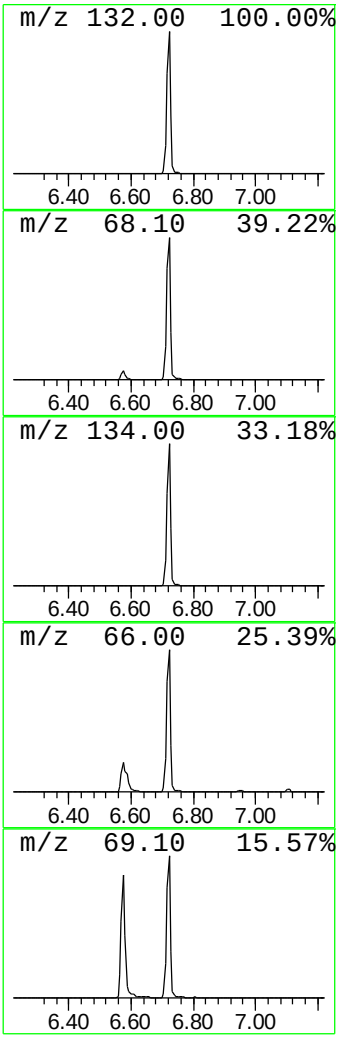
****

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	64.15 ng	1216620	1,4-Dichlorobenzene-d4	6.95

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	12
3	Xenon	132	Xe	007440-63-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
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Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

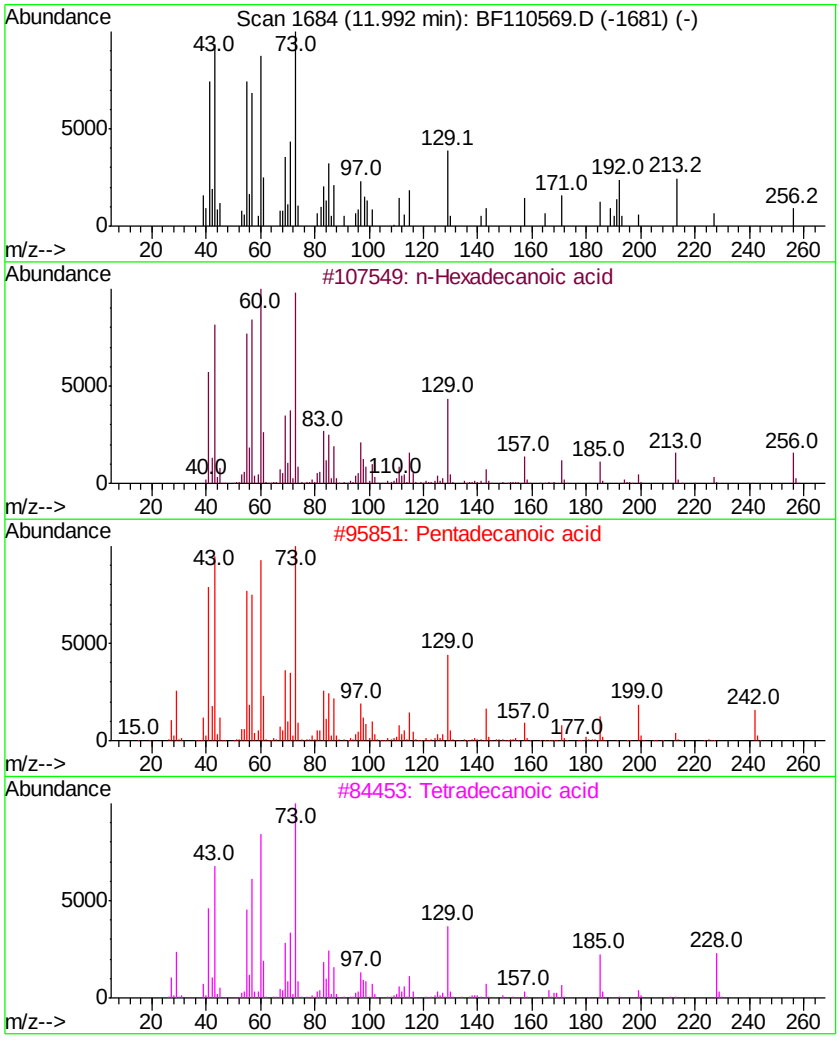
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

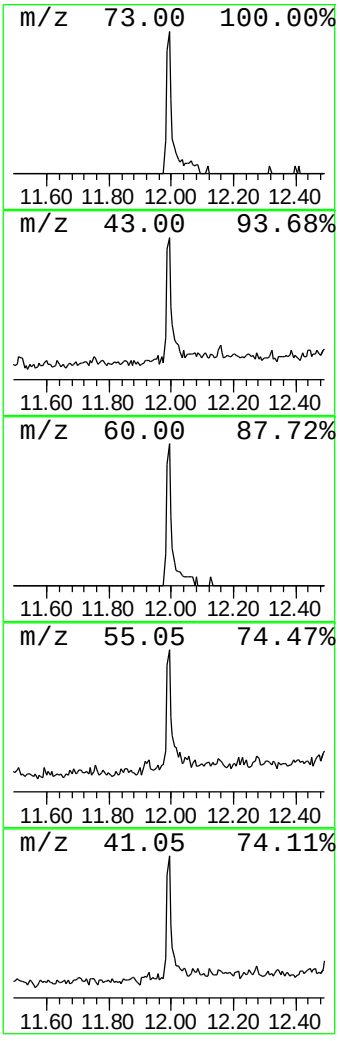
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	3.93 ng	71040	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110569.D
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Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

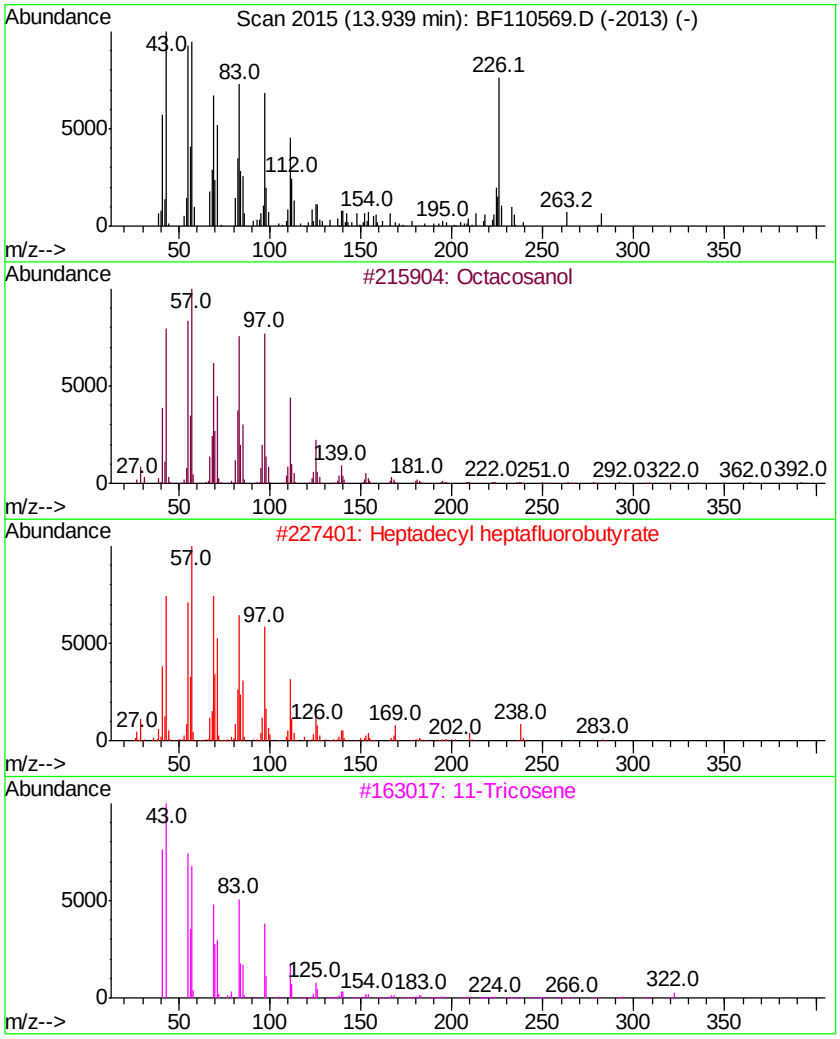
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

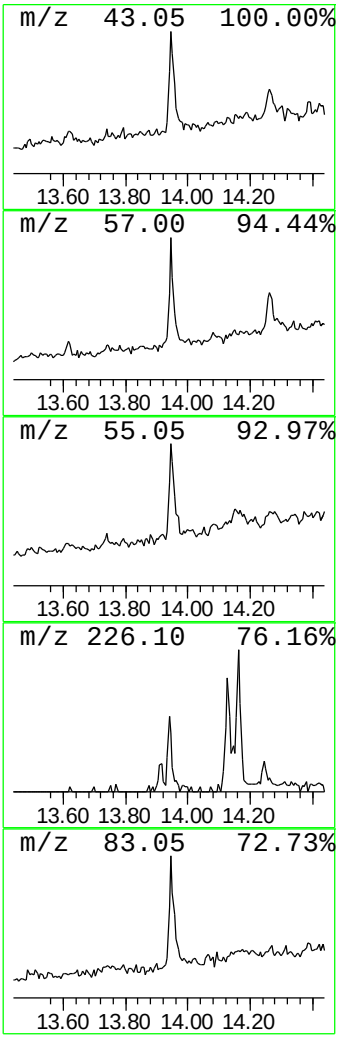
****

Peak Number 6 Octacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	4.56 ng	126882	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	87
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3	11-Tricosene	322	C23H46	052078-56-5	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	Trichloroacetic acid, 4-hexadecy...	386	C18H33Cl3O2	1000282-92-4	87





Library Search Compound Report

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Data File : BF110569.D
Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

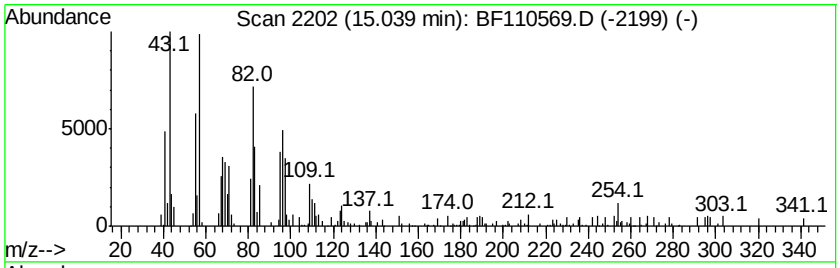
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

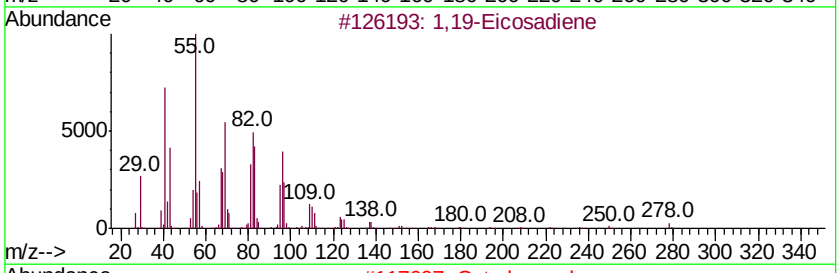
****

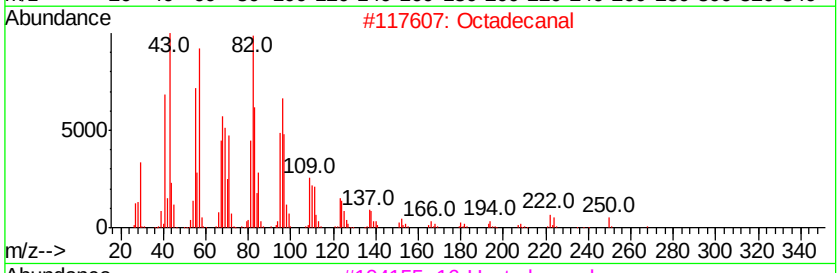
Peak Number 7 1,19-Eicosadiene Concentration Rank 5

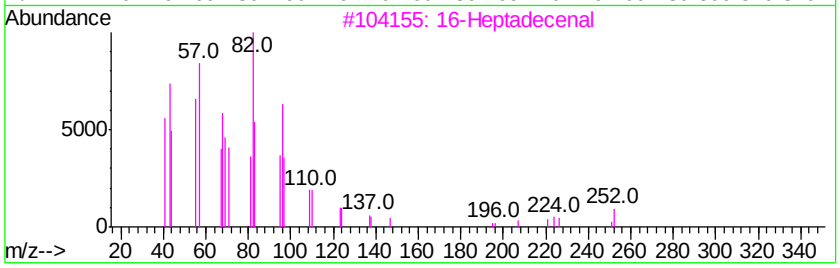
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	7.21 ng	95598	Perylene-d12	15.67

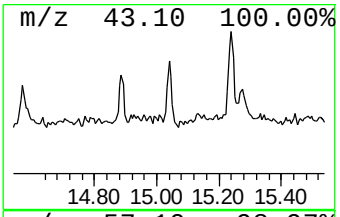
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	91
2	Octadecanal	268	C18H36O	000638-66-4	87
3	16-Heptadecenal	252	C17H32O	1000144-57-9	86
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
5	Pentadecanal-	226	C15H30O	002765-11-9	86

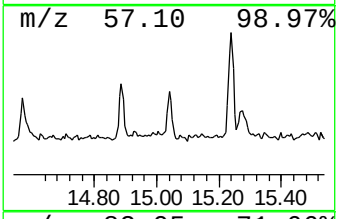


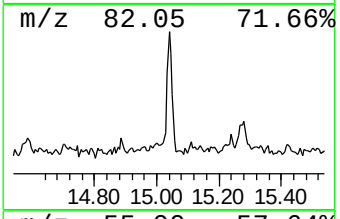


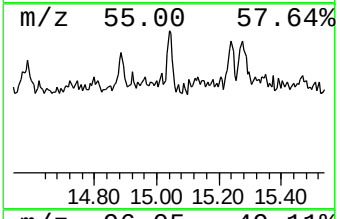


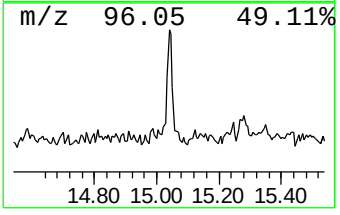












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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

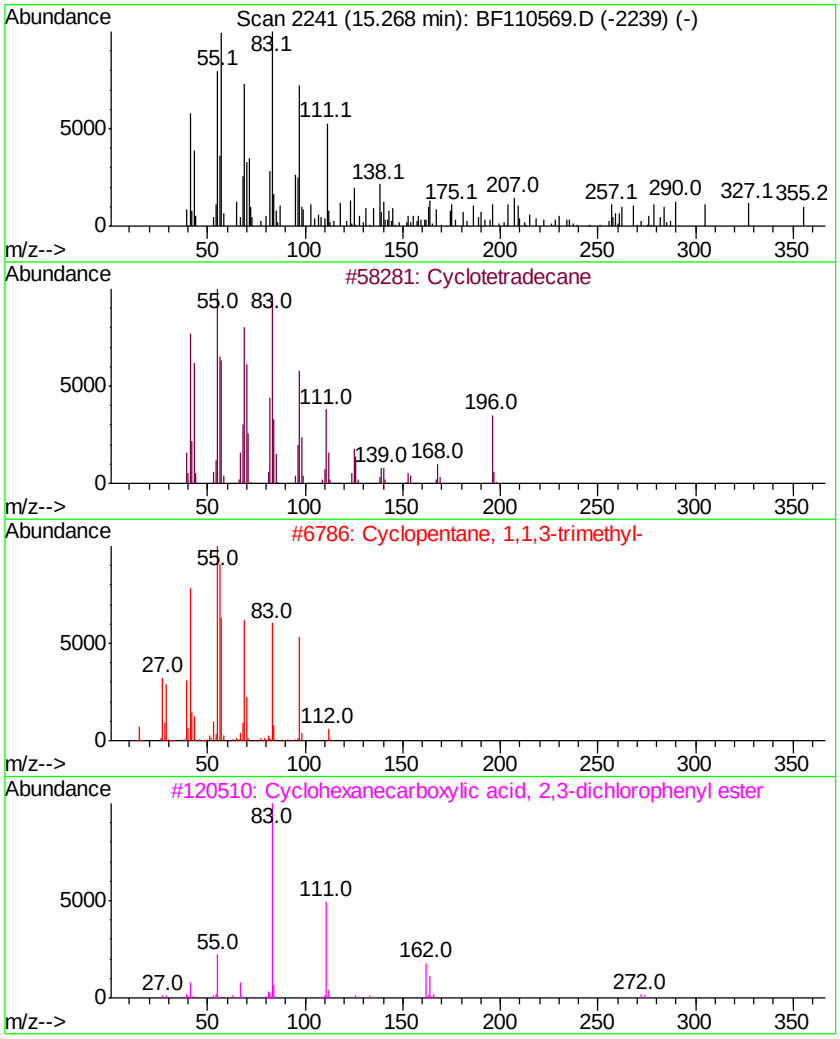
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

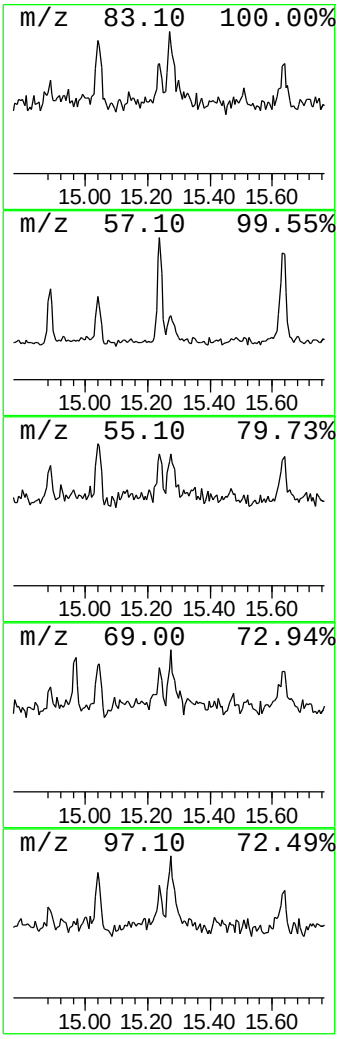
****

Peak Number 8 Cyclotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	4.54 ng	60123	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	58
2	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	43
3	Cyclohexanecarboxylic acid, 2,3-...	272	C13H14Cl2O2	1000330-88-3	38
4	Octacosanol	410	C28H58O	000557-61-9	38
5	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	27





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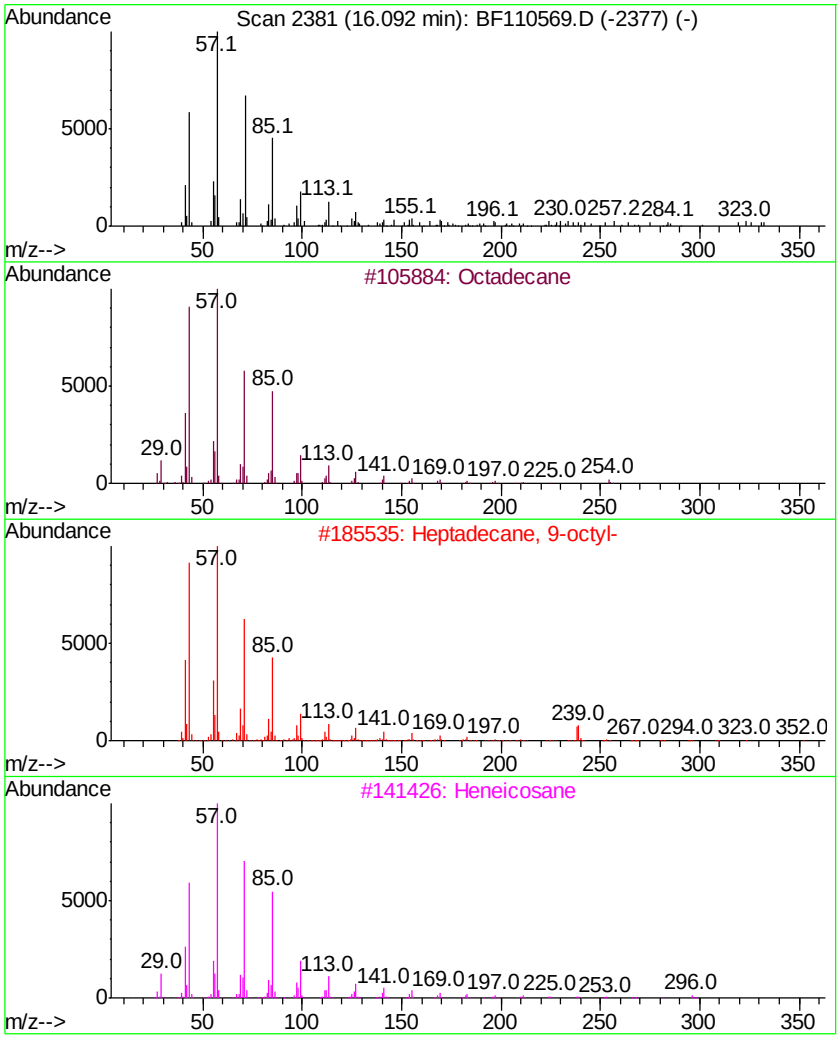
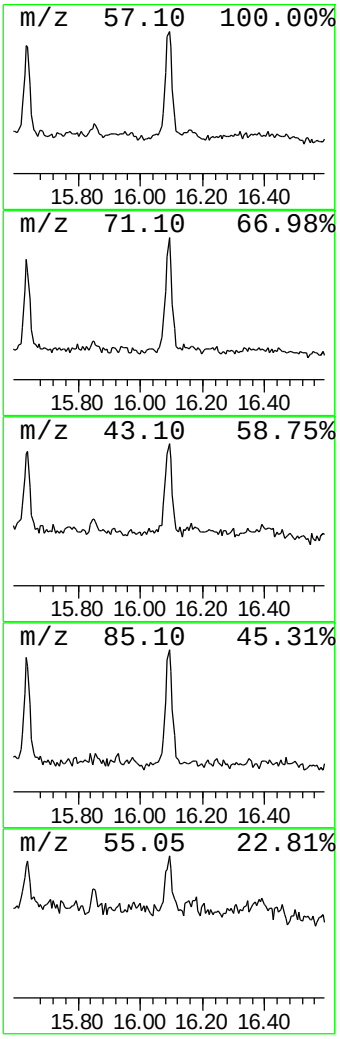
Peak Number 9 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	11.66 ng	154553	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	86
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Octacosane	394	C28H58	000630-02-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110718\
Data File : BF110569.D
Acq On : 7 Nov 2018 21:28
Operator : JU/SJ
Sample : J5813-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	2.26	16.6	ng	313871	1	6.95	379331	20.0
2-Pentanone, 4-hy...	5.19	2.5	ng	47929	1	6.95	379331	20.0
unknown6.72	6.72	64.2	ng	1216620	1	6.95	379331	20.0
n-Hexadecanoic acid	11.99	3.9	ng	71040	4	11.49	361368	20.0
Octacosanol	13.94	4.6	ng	126882	5	14.14	556895	20.0
1,19-Eicosadiene	15.04	7.2	ng	95598	6	15.67	265100	20.0
Cyclotetradecane	15.27	4.5	ng	60123	6	15.67	265100	20.0
Octadecane	16.09	11.7	ng	154553	6	15.67	265100	20.0