LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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	2.316	32	39	48	rVB	437212	598633	16.80%	2.168%
2	3.598	255	257	271	rBV	49692	83924	2.36%	0.304%
3	5.210	528	531	542	rVB	94738	137959	3.87%	0.500%
4	5.587	590	595	598	rBV	2682080	2769836	77.75%	10.031%
5	6.587	758	765	769	rBV	2583082	3071958	86.23%	11.125%
6	6.728	784	789	792	rBV	2906079	3014904	84.62%	10.918%
7	6.957	824	828	831	rBV	641221	563447	15.82%	2.040%
8	7.110	850	854	858	rBV	2339771	2291398	64.32%	8.298%
9	7.522	918	924	927	rBV	1759170	1898543	53.29%	6.875%
10	8.239	1041	1046	1060	rBV	756635	754006	21.16%	2.731%
11	9.316	1222	1229	1232	rBV	3580921	3562702	100.00%	12.902%
12	9.704	1289	1295	1300	rBV	423206	420216	11.79%	1.522%
13	9.998	1340	1345	1355	rVB	915703	882647	24.77%	3.196%
14	10.104	1360	1363	1366	rVV	58344	43609	1.22%	0.158%
15	10.716	1464	1467	1470	rVB	53199	44088	1.24%	0.160%
16	10.763	1470	1475	1476	rBV	52237	55046	1.55%	0.199%
17	10.792	1476	1480	1483	rBV	2157133	1959004	54.99%	7.094%
18	11.486	1594	1598	1606	rBV	847568	808243	22.69%	2.927%
19	13.074	1863	1868	1871	rBV	2873358	2576328	72.31%	9.330%
20	13.945	2013	2016	2030	rVB	166554	203763	5.72%	0.738%
21	14.133	2044	2048	2054	rBV	527843	492203	13.82%	1.782%
22	14.262	2067	2070	2076	rVB	39725	40390	1.13%	0.146%
23	14.580	2119	2124	2130	rBV2	57139	102510	2.88%	0.371%
24	14.886	2172	2176	2180	rBV	46317	48013	1.35%	0.174%
25	15.039	2199	2202	2207	rVB2	48679	51472	1.44%	0.186%
26	15.239	2231	2236	2239	rBV	61641	73008	2.05%	0.264%
27	15.268	2239	2241	2247	rVB3	25567	38219	1.07%	0.138%
28	15.656	2299	2307	2315	rVB2	372785	550292	15.45%	1.993%
29	15.851	2336	2340	2346	rVB3	28357	38742	1.09%	0.140%
30	16.092	2376	2381	2387	rVB	69392	98262	2.76%	0.356%
31	16.156	2387	2392	2399	rBV7	26148	55180	1.55%	0.200%
32	16.621	2466	2471	2477	rBV2	24443	41343	1.16%	0.150%
33	17.245	2573	2577	2585	rVB3	22917	45568	1.28%	0.165%
34	17.356	2590	2596	2603	rBV5	70670	144762	4.06%	0.524%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

35	17.803	2667	2672	2682	rVB5	22154	53869	1.51%	0.195%

Sum of corrected areas: 27614087

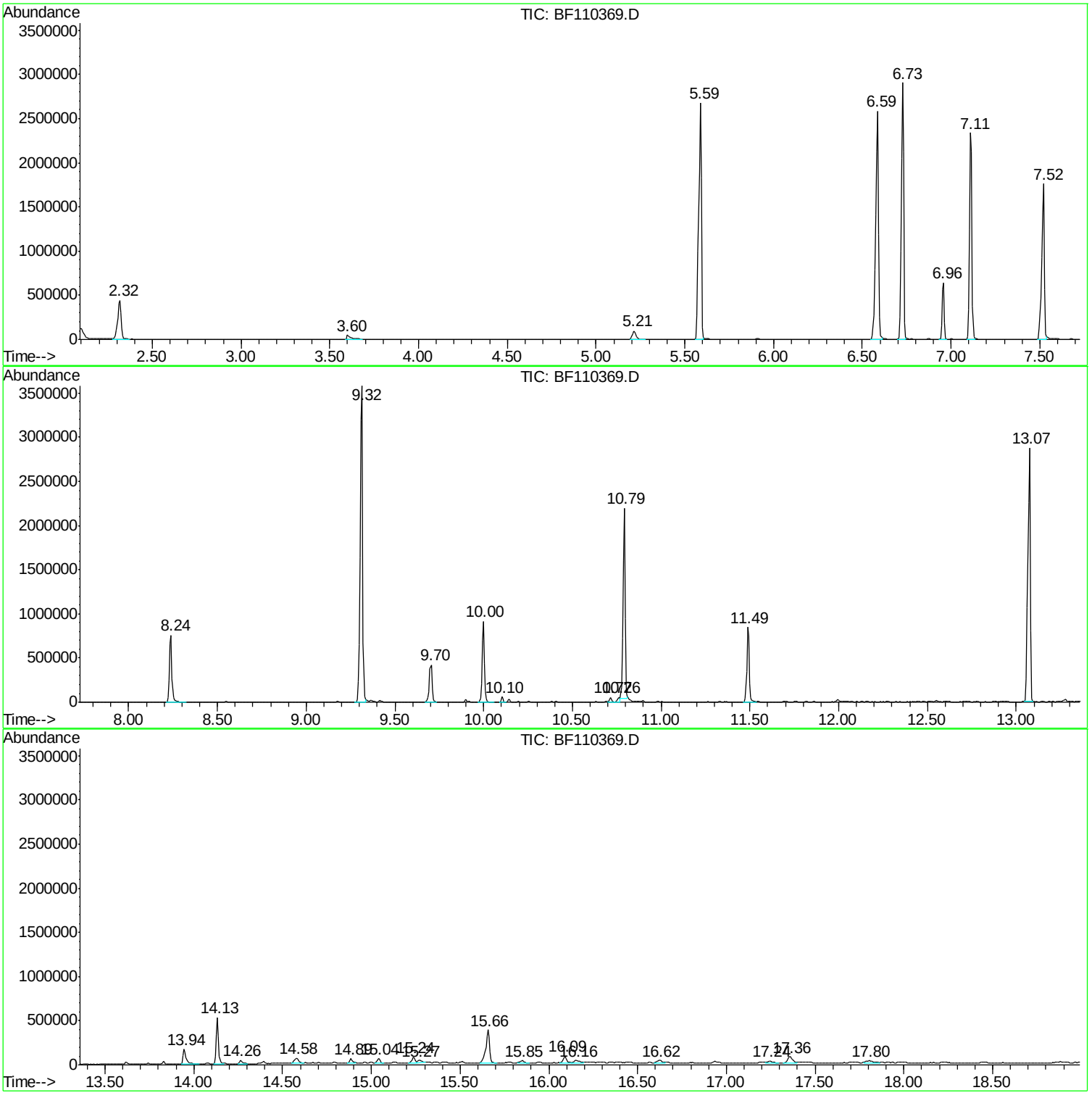
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

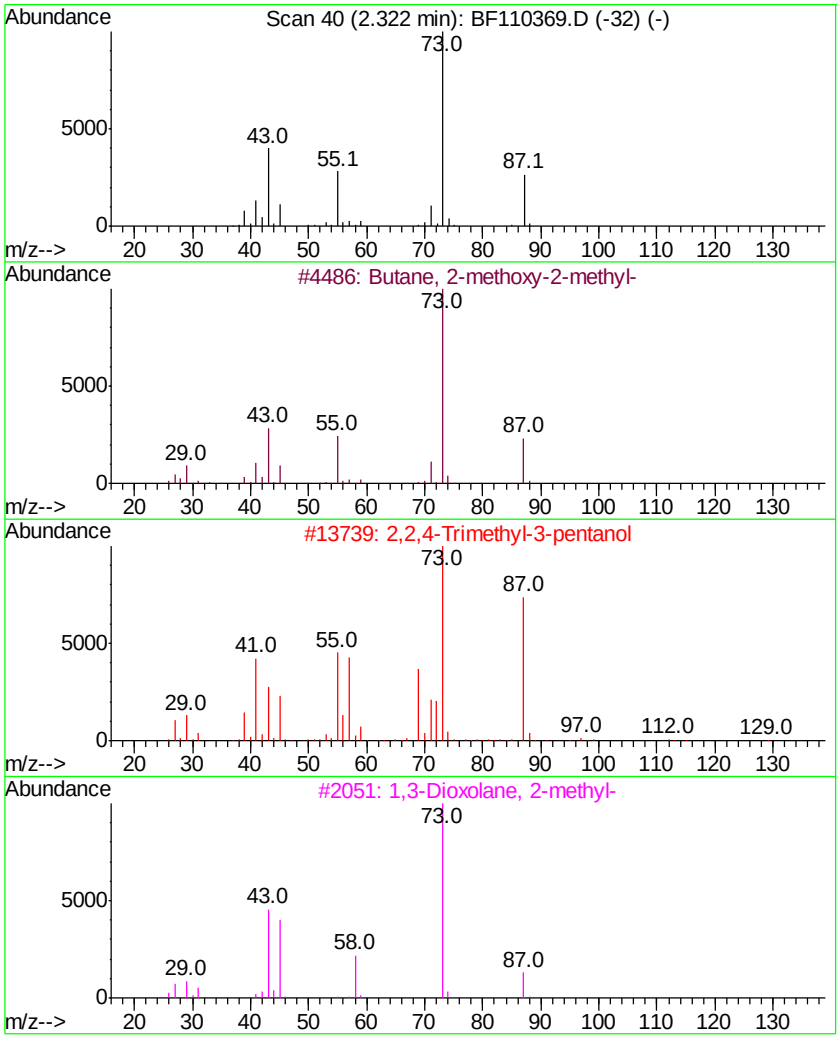
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

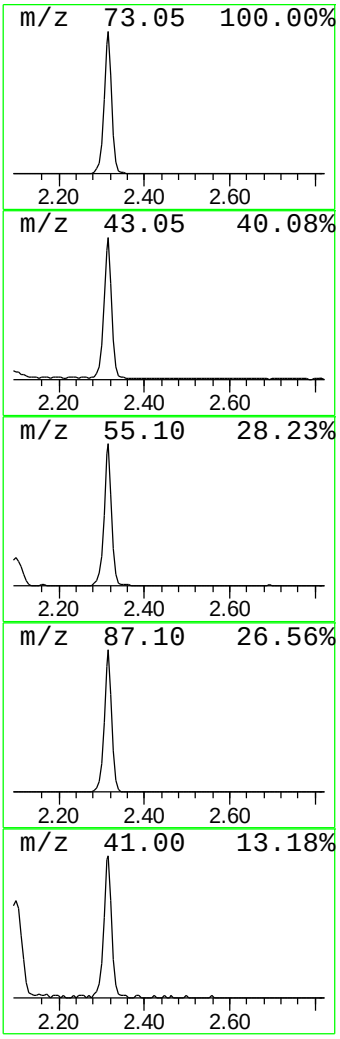
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	21.25 ng	598633	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
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	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

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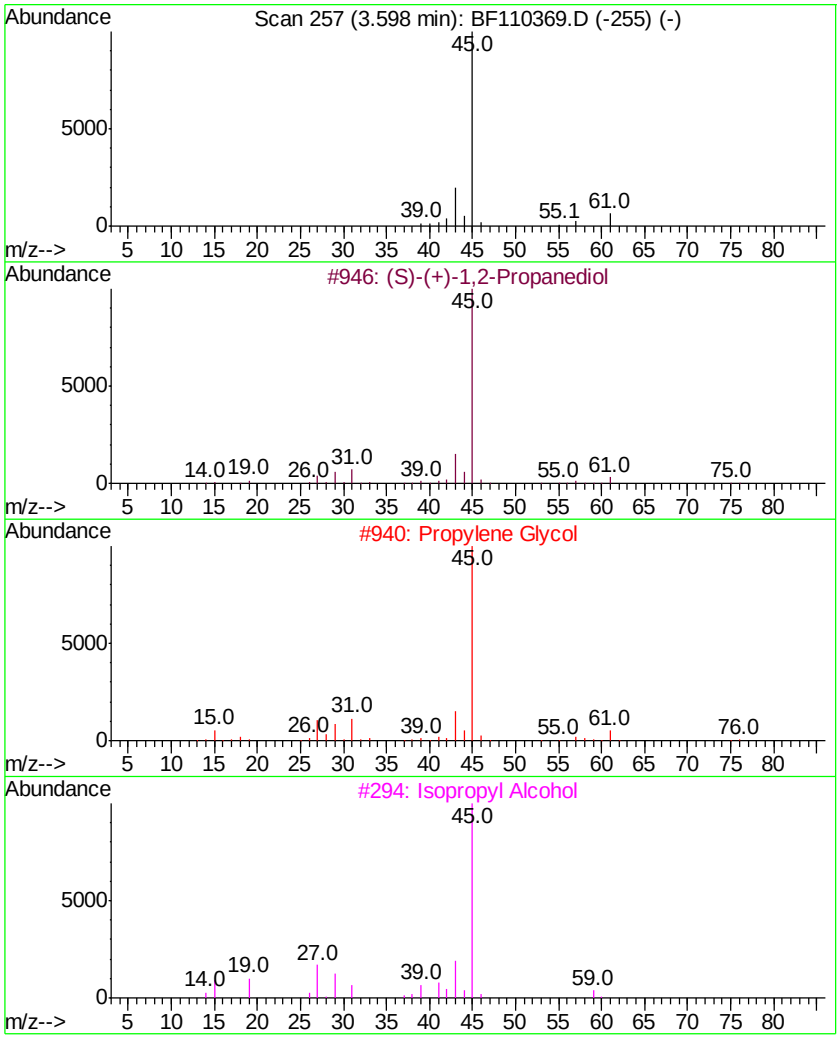
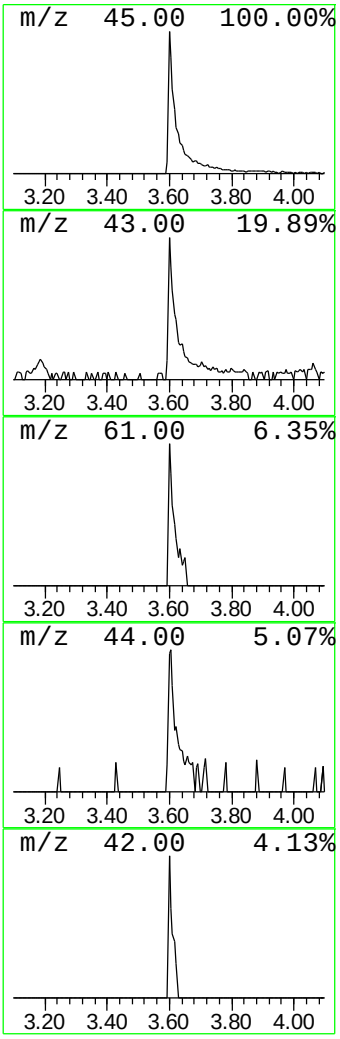
Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	2.98 ng	83924	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Formamide	45	CH3NO	000075-12-7	5
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	4





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

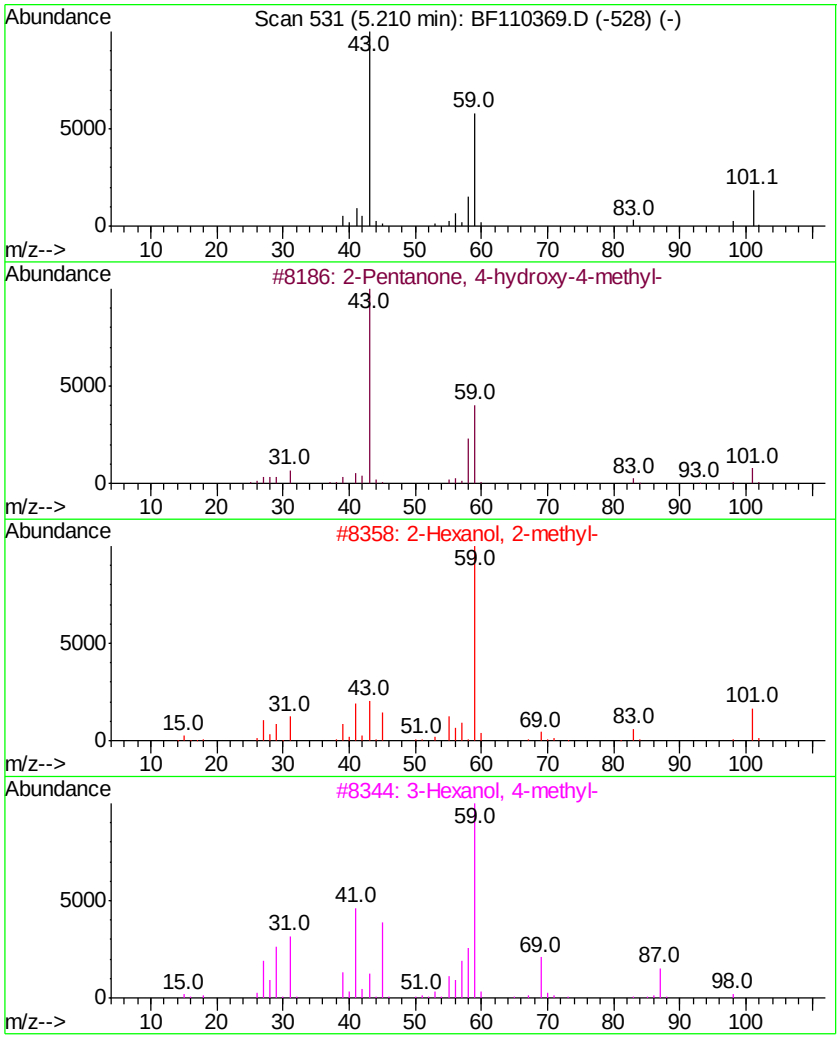
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

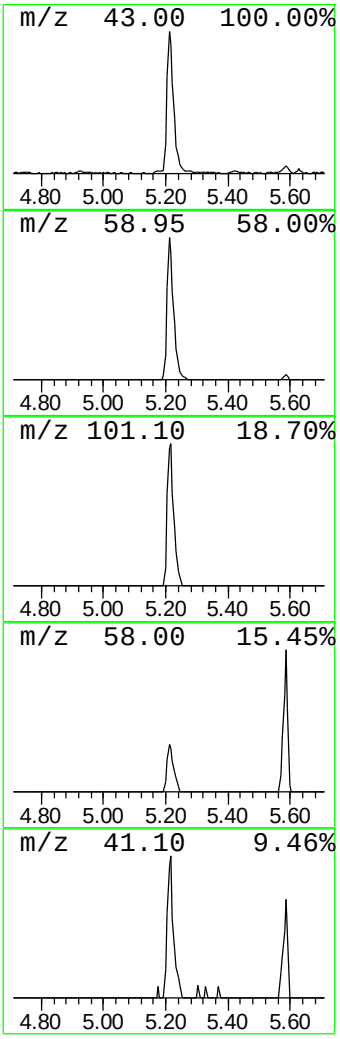
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	4.90 ng	137959	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

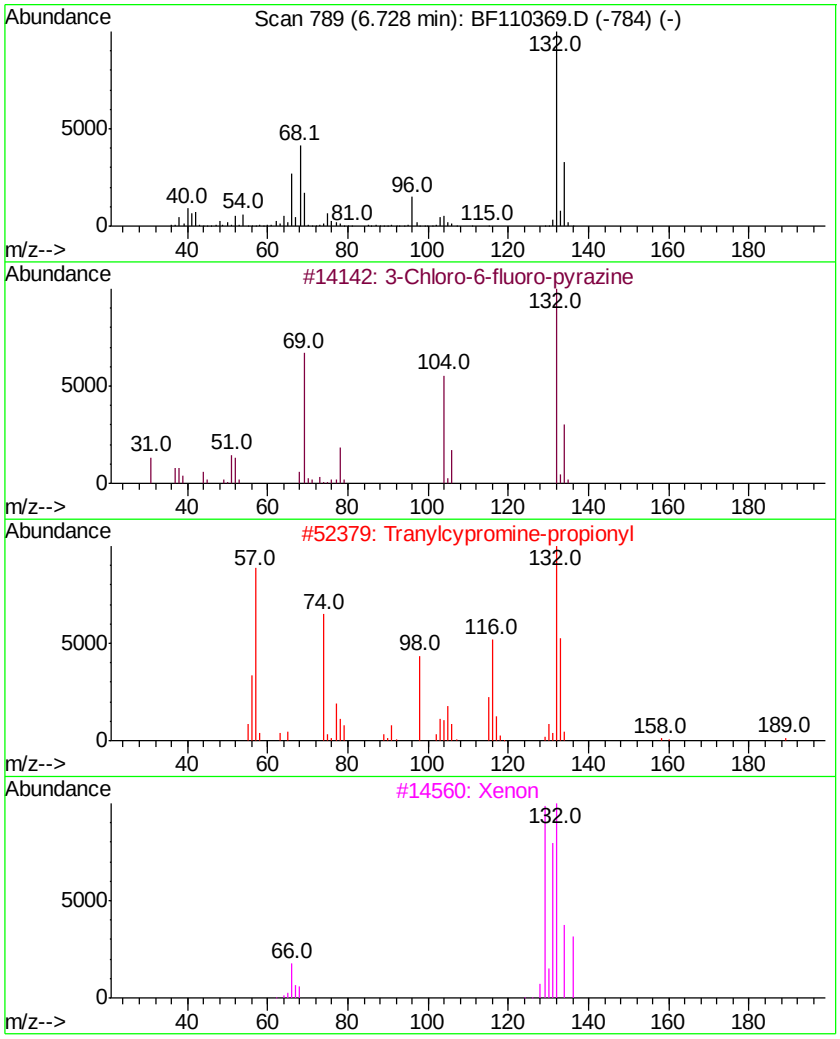
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

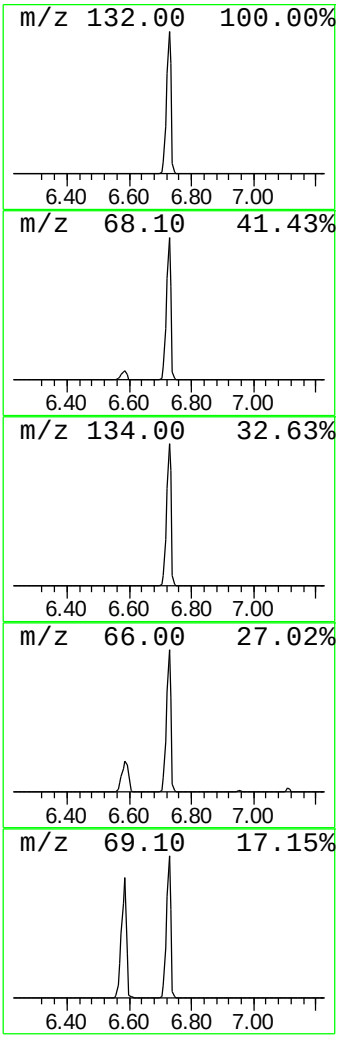
****

Peak Number 4 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	107.02 ng	3014900	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

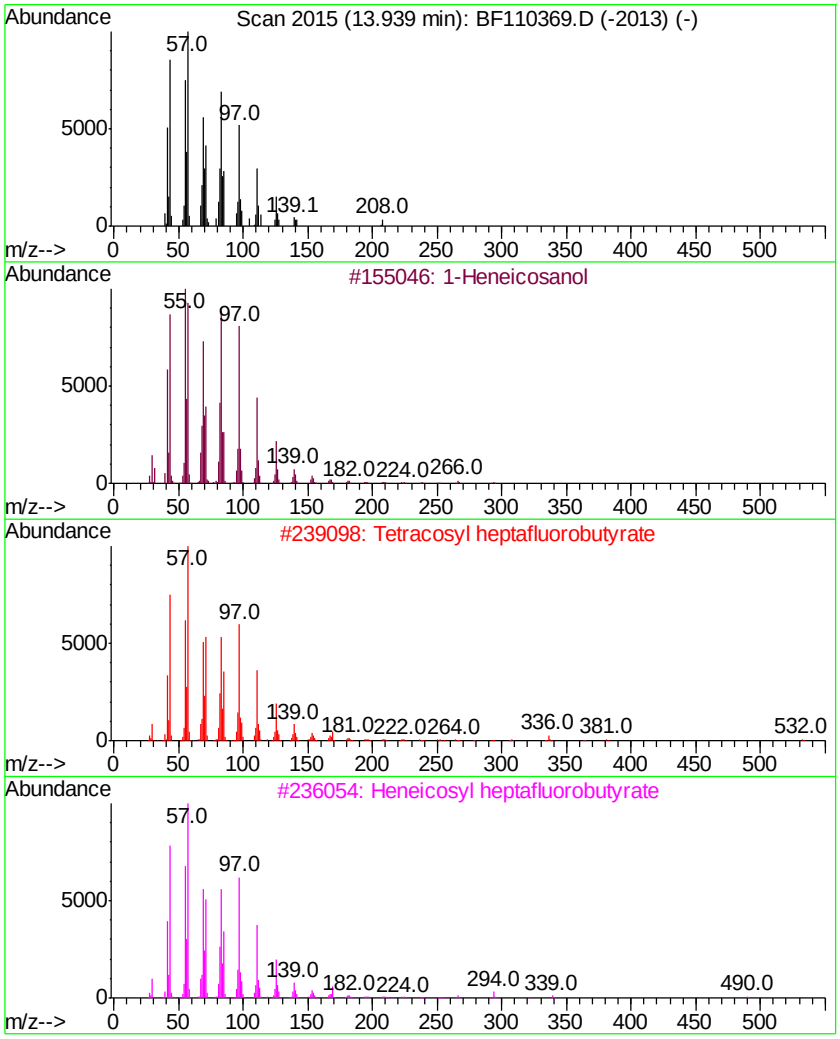
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

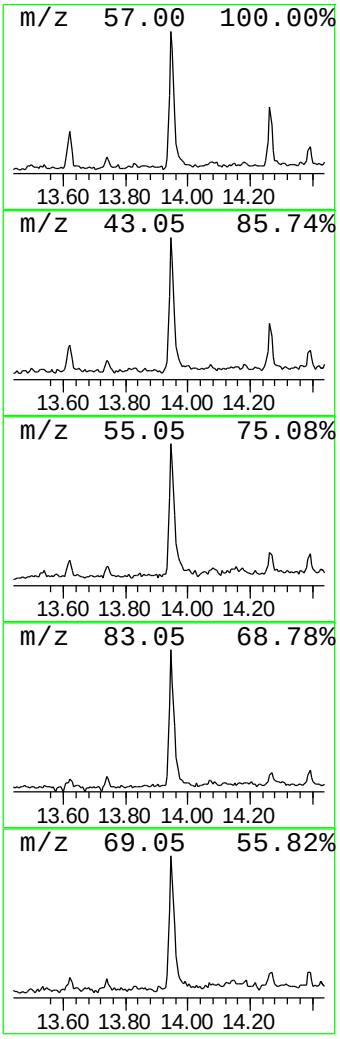
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	8.28 ng	203763	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

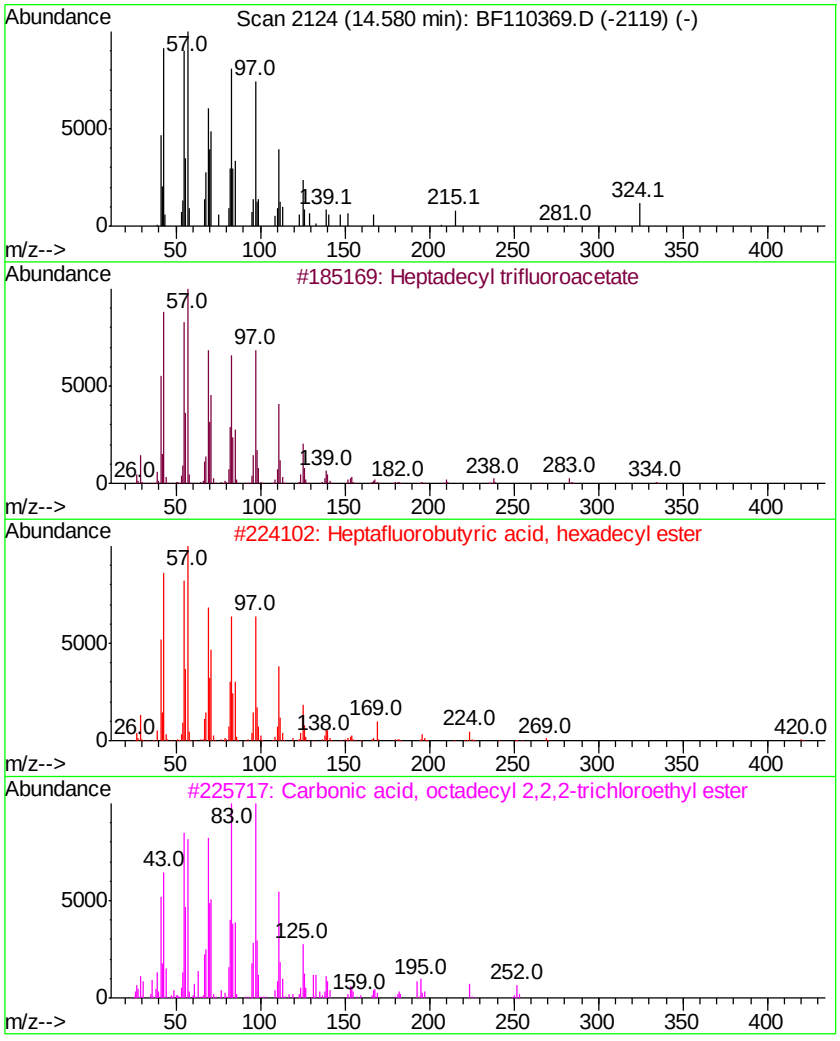
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

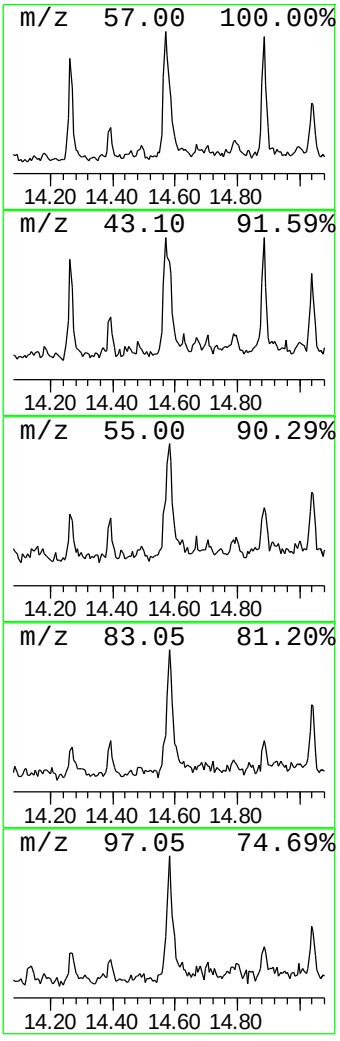
****

Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	4.17 ng	102510	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

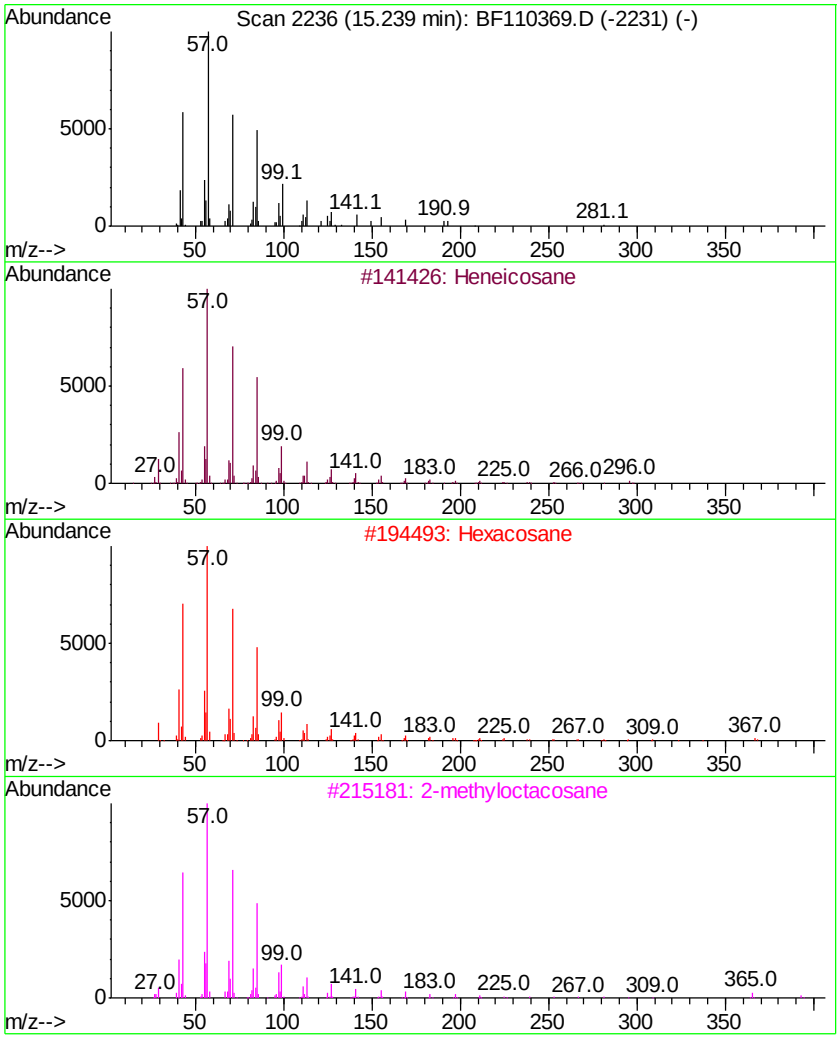
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

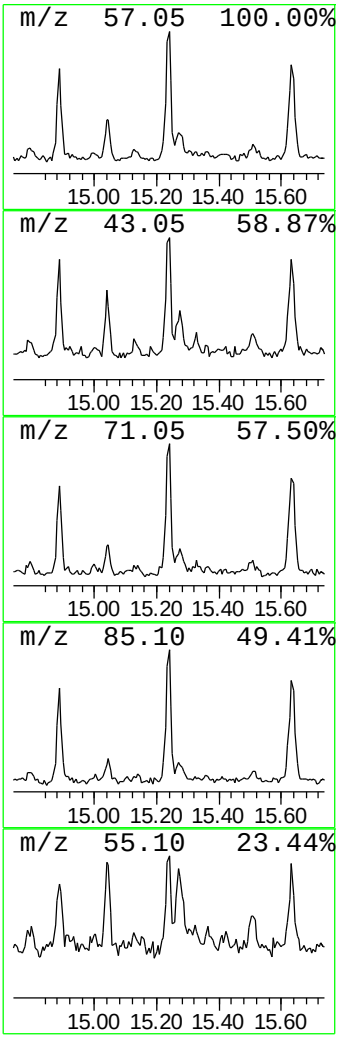
****

Peak Number 8 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.65 ng	73008	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Triacontane	422	C30H62	000638-68-6	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

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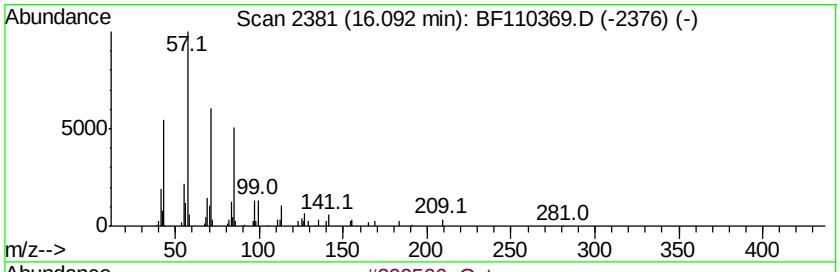
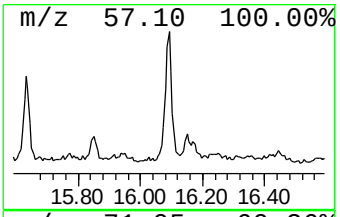
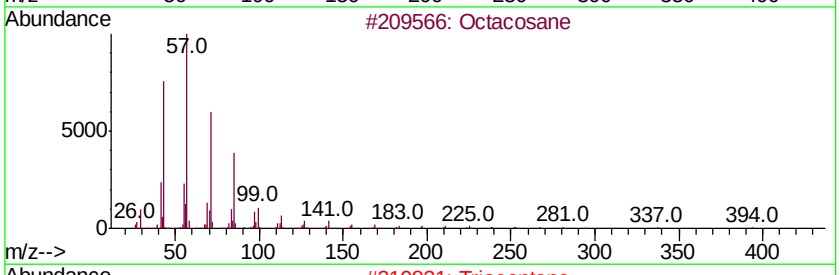
Peak Number 9 Octacosane Concentration Rank 8

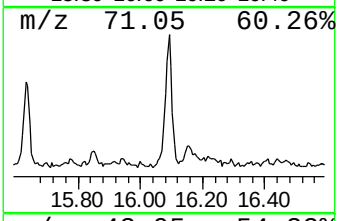
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	3.57 ng	98262	Perylene-d12	15.66

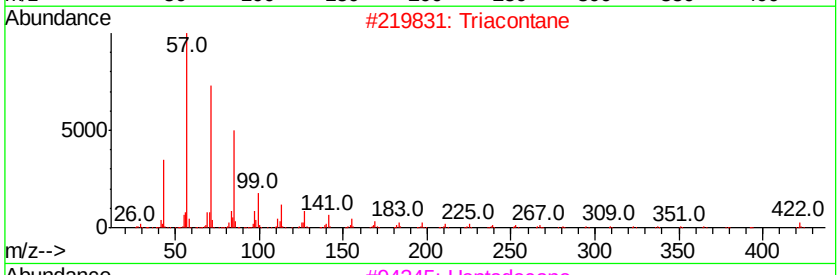
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Triacontane	422	C30H62	000638-68-6	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Octadecane	254	C18H38	000593-45-3	83
5	Heptacosane	380	C27H56	000593-49-7	81

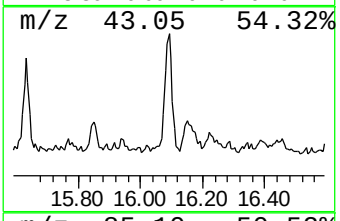


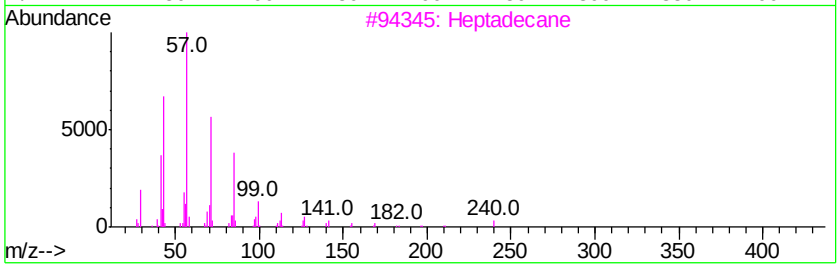


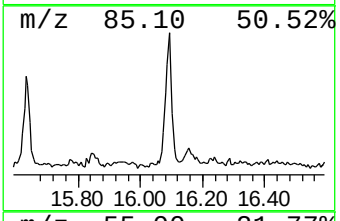


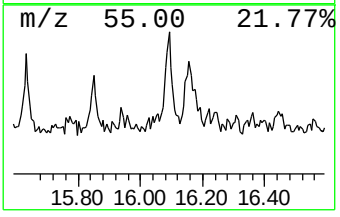












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

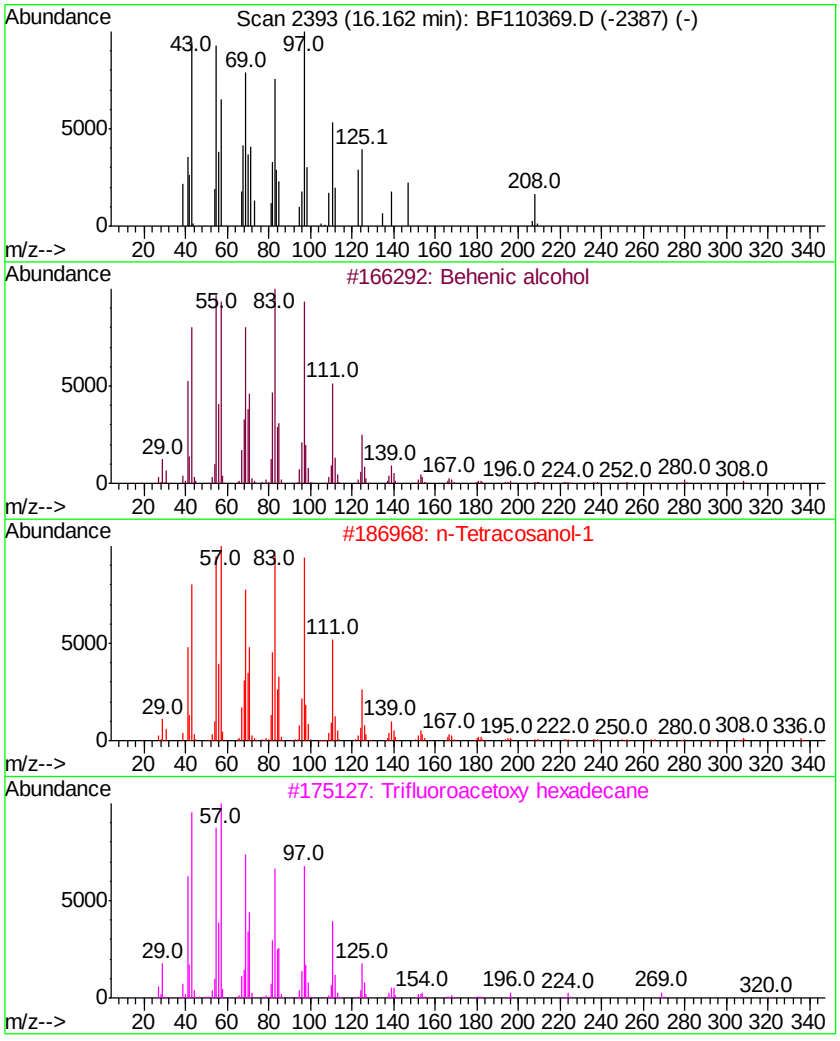
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

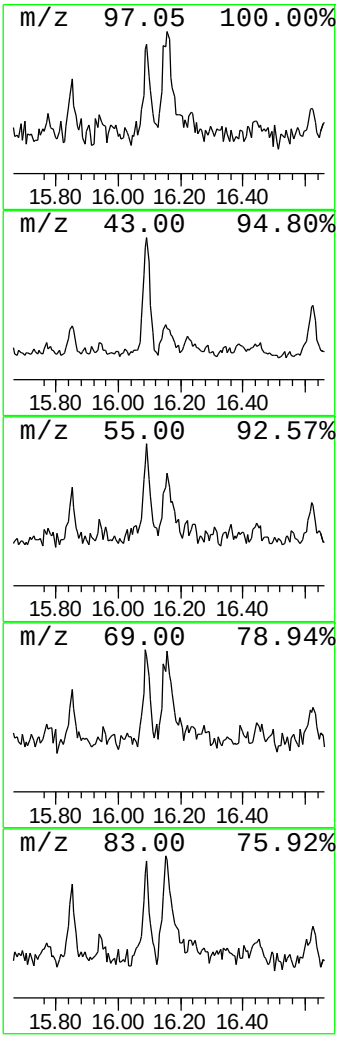
****

Peak Number 10 Behenic alcohol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	2.01 ng	55180	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	87
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	83
4	1-Heneicosanol	312	C21H44O	015594-90-8	83
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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

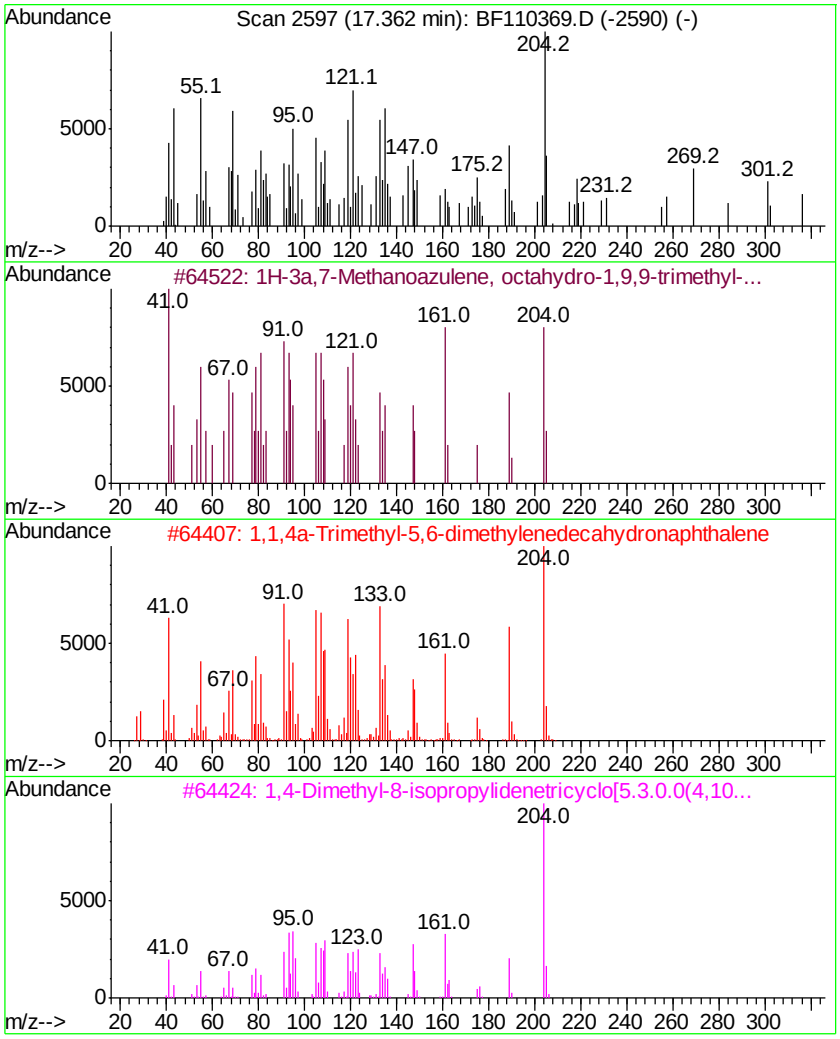
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

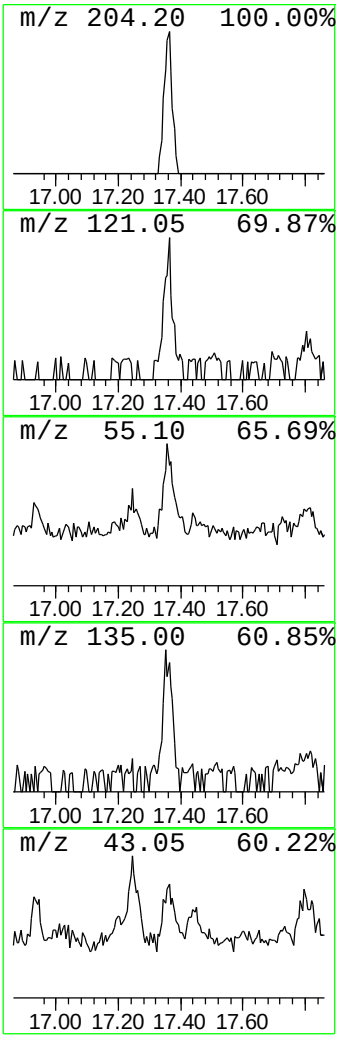
****

Peak Number 11 1H-3a,7-Methanoazulene, oct... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.36	5.26 ng	144762	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	86
2	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	83
3	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	68
4	Solavetivone	218	C15H22O	054878-25-0	66
5	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110118\
Data File : BF110369.D
Acq On : 1 Nov 2018 15:28
Operator : JU/SJ
Sample : J5741-51
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13

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...	2.32	21.3	ng	598633	1	6.96	563447	20.0
(S)-(+)-1,2-Propa...	3.60	3.0	ng	83924	1	6.96	563447	20.0
2-Pentanone, 4-hy...	5.21	4.9	ng	137959	1	6.96	563447	20.0
unknown6.73	6.73	107.0	ng	3014900	1	6.96	563447	20.0
1-Heneicosanol	13.94	8.3	ng	203763	5	14.13	492203	20.0
Heptadecyl triflu...	14.58	4.2	ng	102510	5	14.13	492203	20.0
Heneicosane	15.24	2.6	ng	73008	6	15.66	550292	20.0
Octacosane	16.09	3.6	ng	98262	6	15.66	550292	20.0
Behenic alcohol	16.16	2.0	ng	55180	6	15.66	550292	20.0
1H-3a,7-Methanoaz...	17.36	5.3	ng	144762	6	15.66	550292	20.0