LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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	2.310	31	38	48	rVB	469056	626929	19.44%	2.452%
2	3.593	255	256	270	rBV	41123	81033	2.51%	0.317%
3	5.210	527	531	541	rVB	93858	131457	4.08%	0.514%
4	5.587	590	595	598	rBV	2616102	2655336	82.32%	10.385%
5	6.587	759	765	769	rBV	2457917	2896804	89.81%	11.329%
6	6.728	784	789	792	rBV	2915000	2860065	88.67%	11.185%
7	6.957	824	828	831	rBV	585447	523980	16.24%	2.049%
8	7.110	850	854	858	rBV	2215255	2182417	67.66%	8.535%
9	7.522	918	924	927	rBV	1689411	1788552	55.45%	6.995%
10	8.239	1041	1046	1059	rBV	684408	691625	21.44%	2.705%
11	9.316	1222	1229	1232	rBV	3213013	3225625	100.00%	12.615%
12	9.704	1290	1295	1306	rVB	383316	369791	11.46%	1.446%
13	9.998	1340	1345	1352	rBV	817418	766722	23.77%	2.999%
14	10.792	1475	1480	1483	rBV	1945247	1873187	58.07%	7.326%
15	11.486	1594	1598	1607	rBV	787603	742537	23.02%	2.904%
16	13.074	1863	1868	1871	rBV	2424567	2338168	72.49%	9.144%
17	13.945	2013	2016	2022	rBV	141042	160921	4.99%	0.629%
18	14.133	2044	2048	2053	rBV	504897	453529	14.06%	1.774%
19	14.263	2067	2070	2078	rBV	42202	54493	1.69%	0.213%
20	14.568	2119	2122	2128	rBV3	42598	70388	2.18%	0.275%
21	14.792	2157	2160	2165	rVB4	26234	33388	1.04%	0.131%
22	14.886	2172	2176	2179	rBV	49790	52676	1.63%	0.206%
23	15.239	2232	2236	2239	rBV	62698	75102	2.33%	0.294%
24	15.510	2279	2282	2290	rVB4	22018	33676	1.04%	0.132%
25	15.657	2299	2307	2319	rVB2	346149	553737	17.17%	2.166%
26	16.092	2376	2381	2388	rBV	59015	89928	2.79%	0.352%
27	16.374	2426	2429	2437	rVB7	18992	38774	1.20%	0.152%
28	16.627	2467	2472	2476	rBV2	28493	48298	1.50%	0.189%
29	16.833	2503	2507	2513	rVB3	25139	47302	1.47%	0.185%
30	17.245	2572	2577	2587	rVB4	19685	48620	1.51%	0.190%
31	17.356	2591	2596	2605	rBV9	24026	54917	1.70%	0.215%

Sum of corrected areas: 25569977

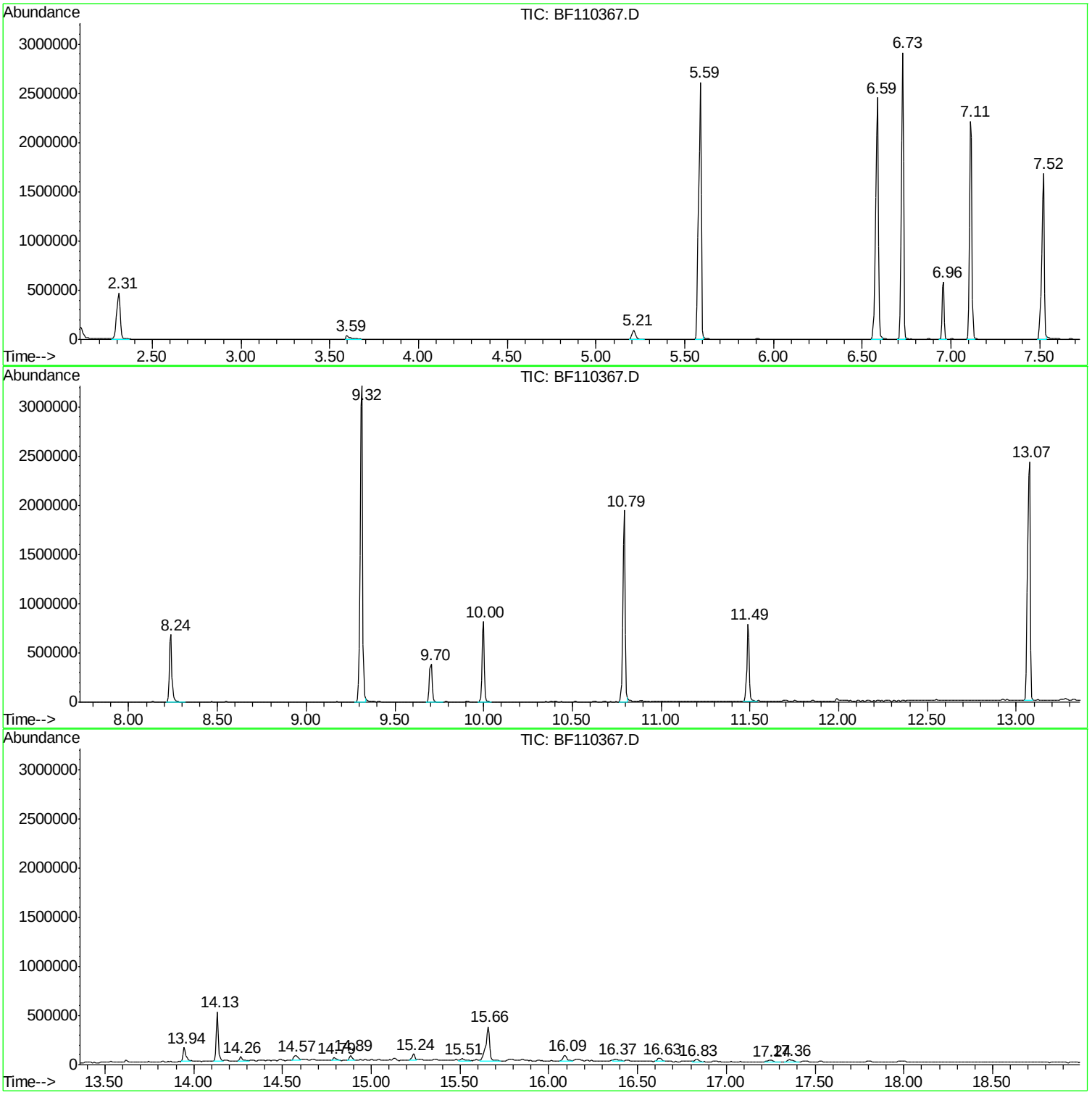
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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

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Data File : BF110367.D
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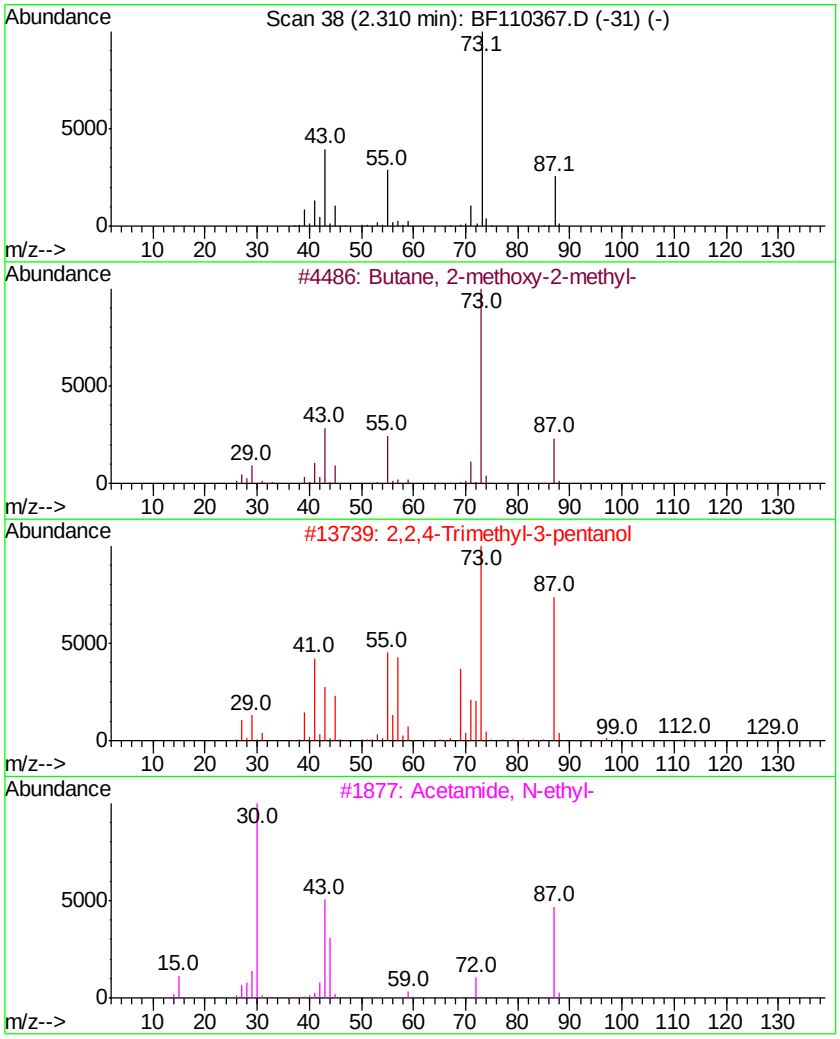
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

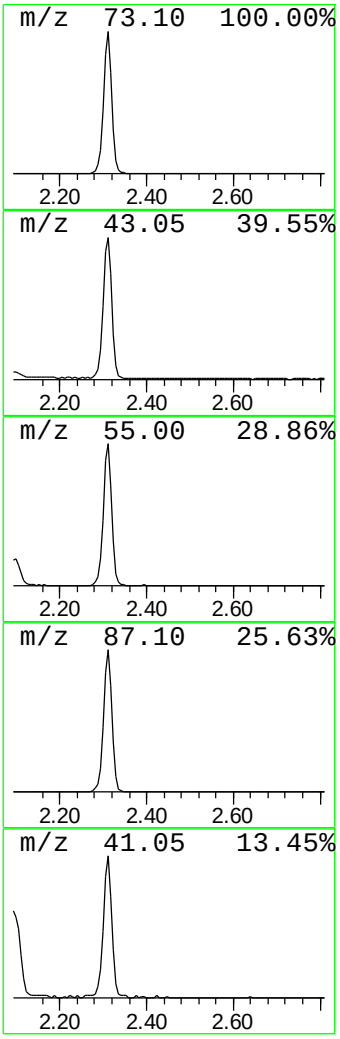
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	23.93 ng	626929	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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Library Search Compound Report

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Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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

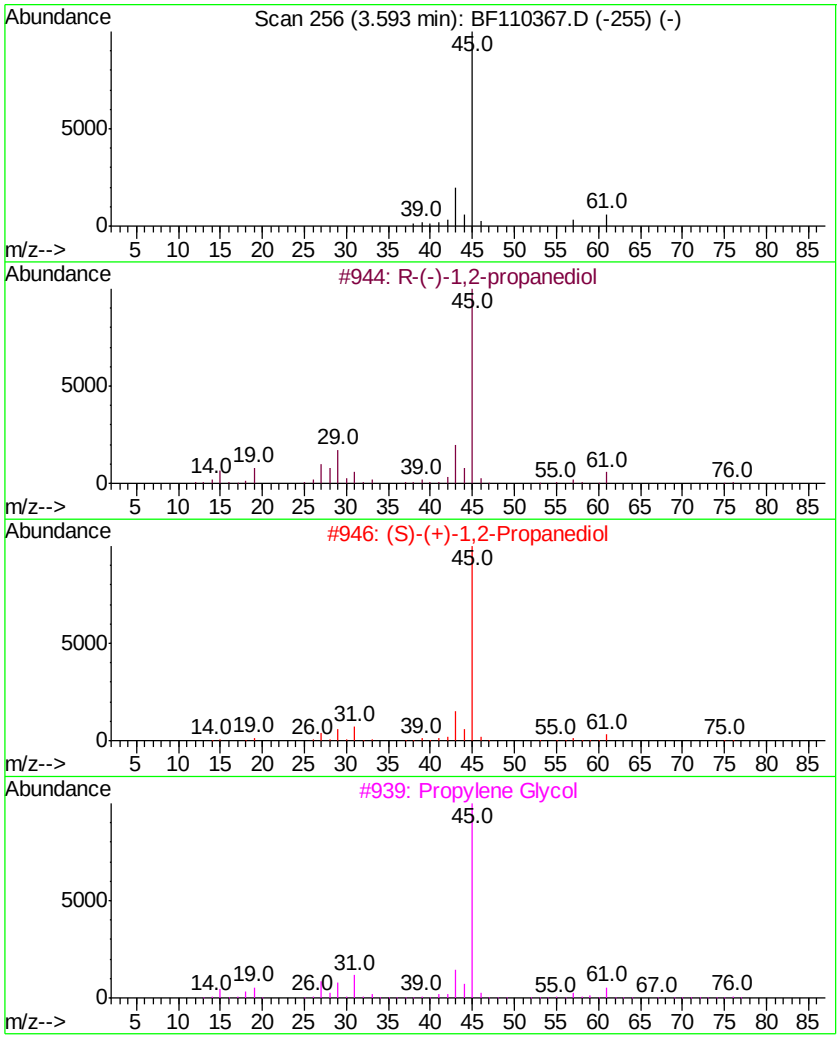
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

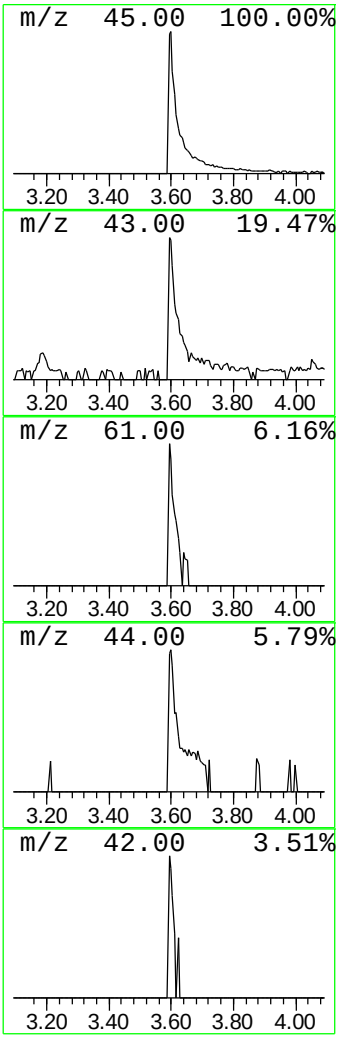
****

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	3.09 ng	81033	1,4-Dichlorobenzene-d4	6.96

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





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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

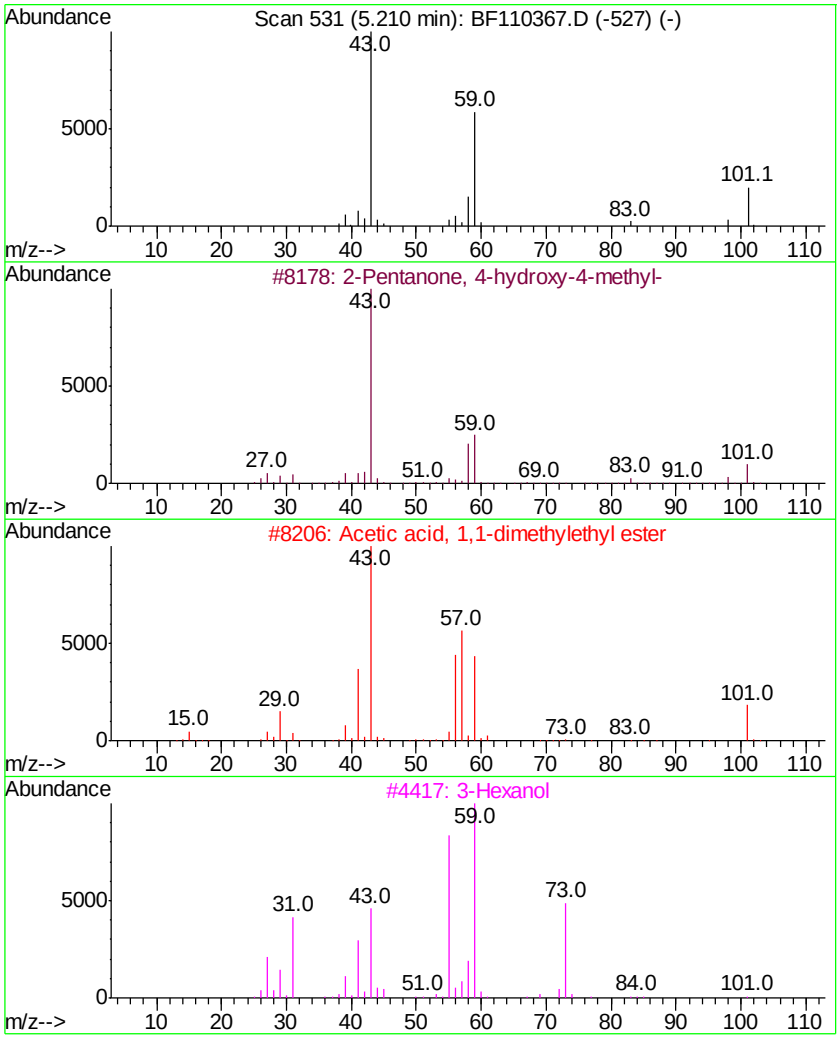
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

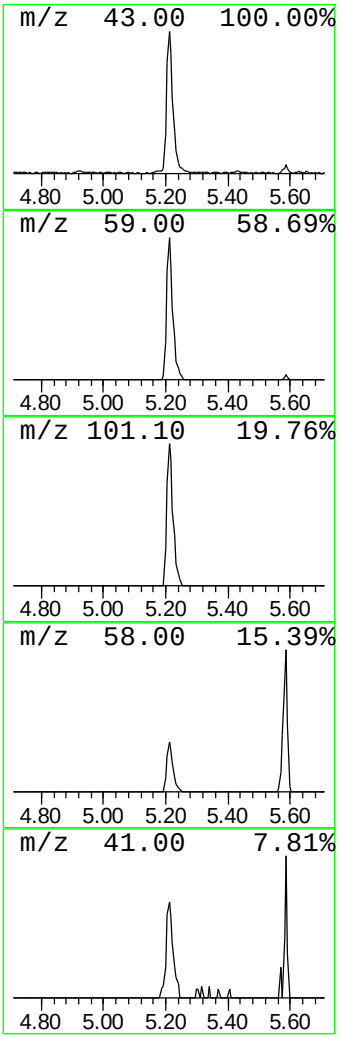
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	5.02 ng	131457	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	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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

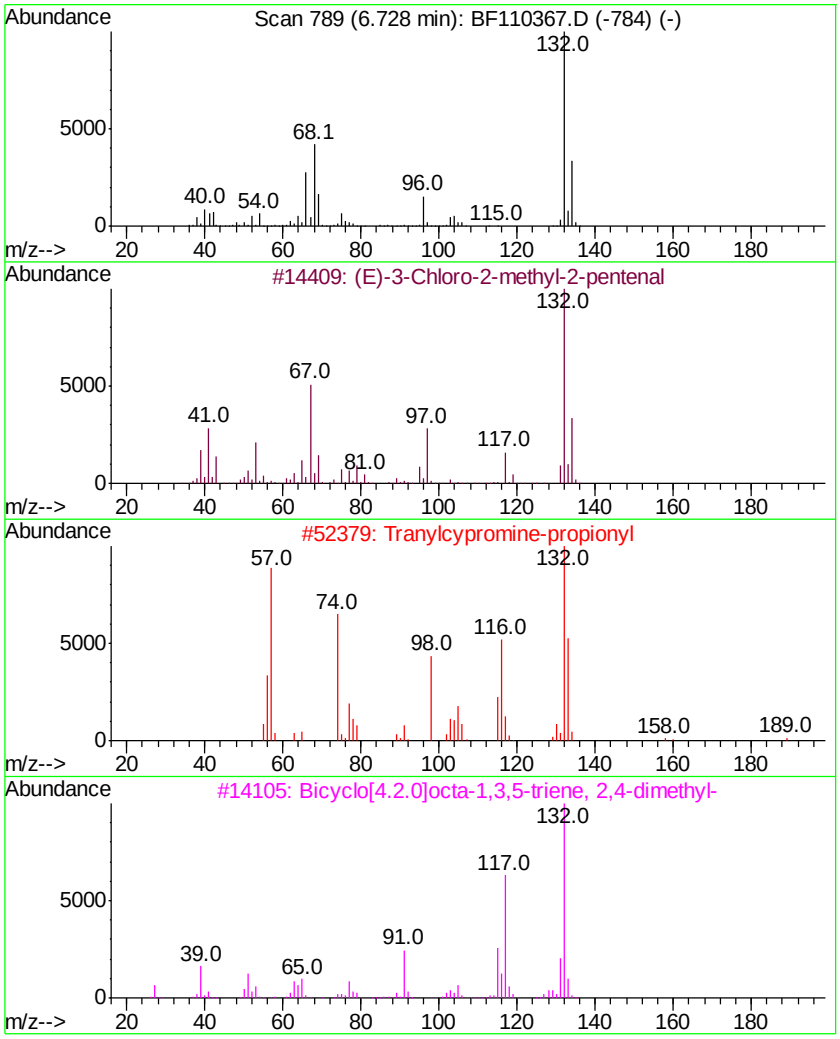
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

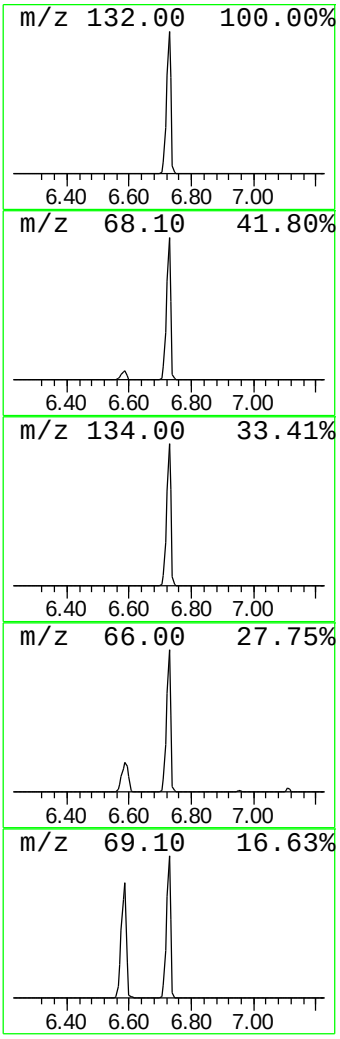
****

Peak Number 4 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	109.17 ng	2860070	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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

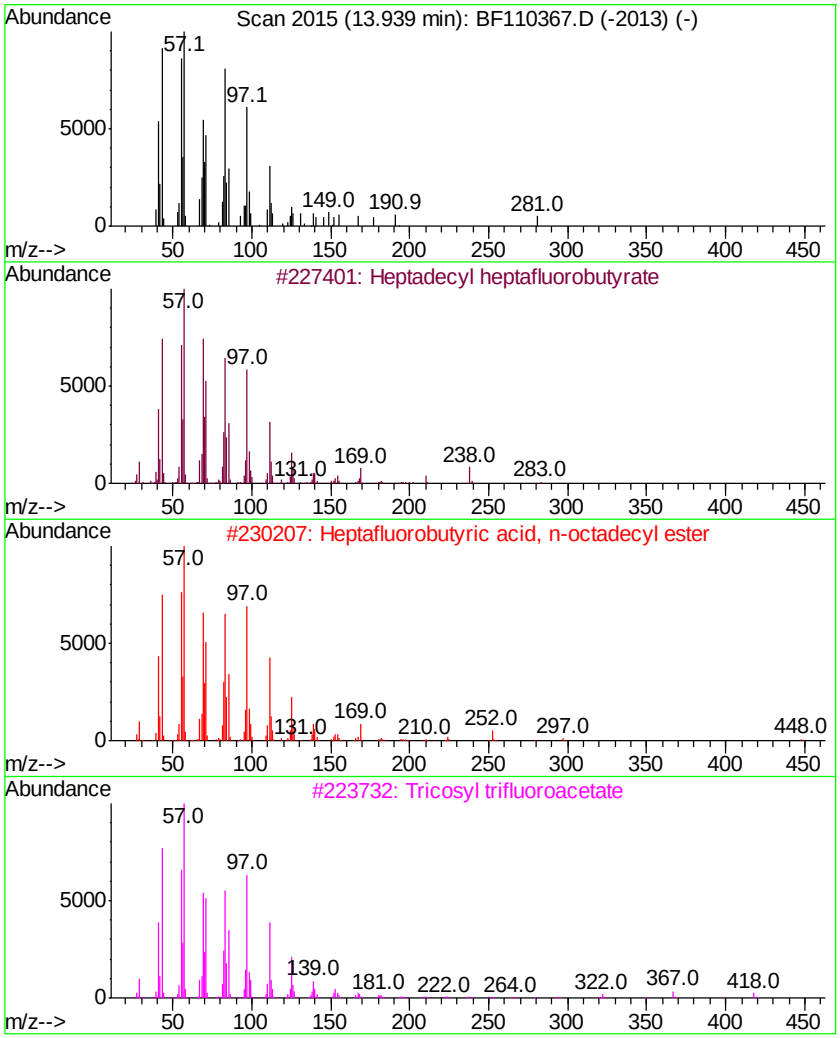
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

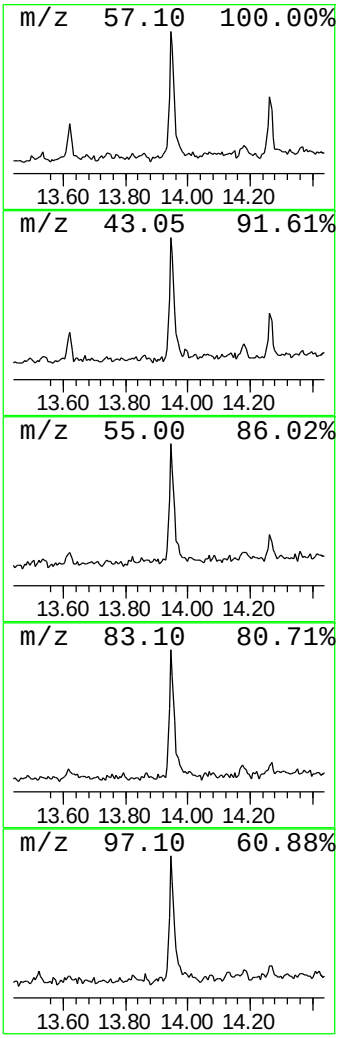
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	7.10 ng	160921	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91





Library Search Compound Report

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Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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
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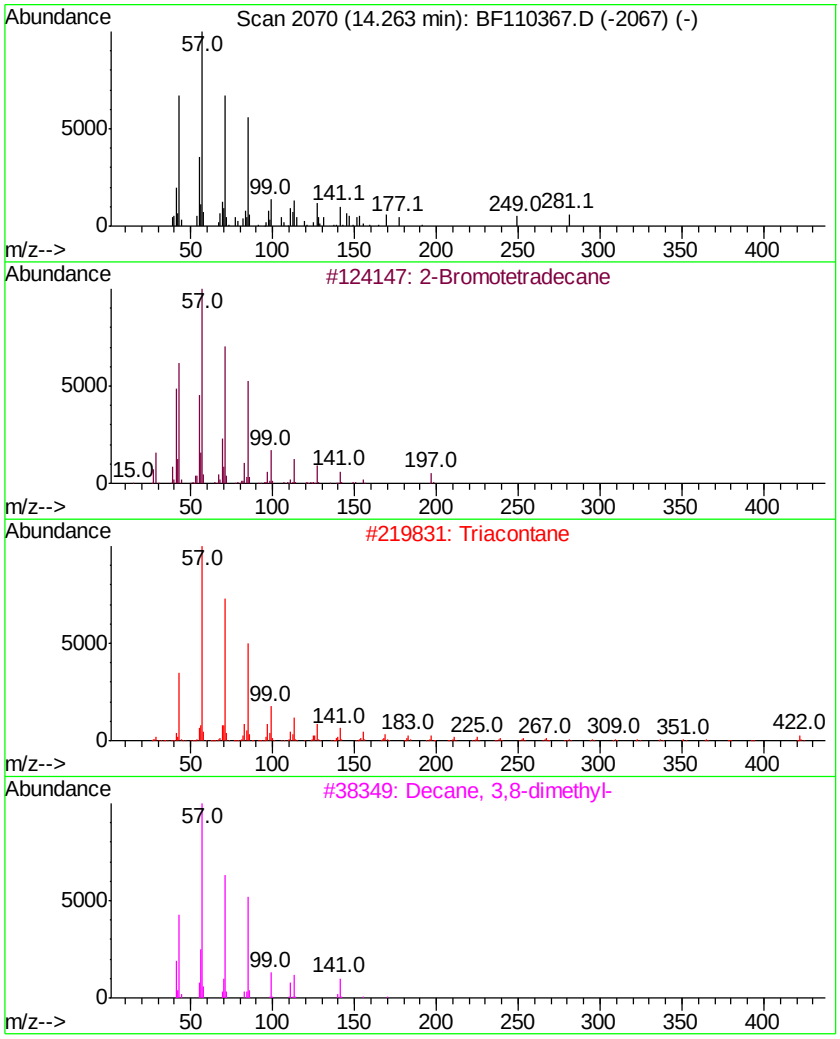
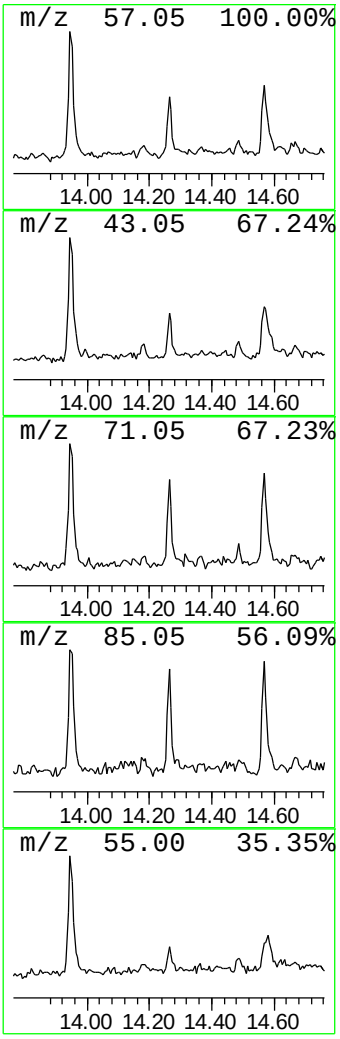
****

Peak Number 7 2-Bromotetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	2.40 ng	54493	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
2	Triacontane	422	C30H62	000638-68-6	86
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	80
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
5	Pentacosane	352	C25H52	000629-99-2	64





Library Search Compound Report

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Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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

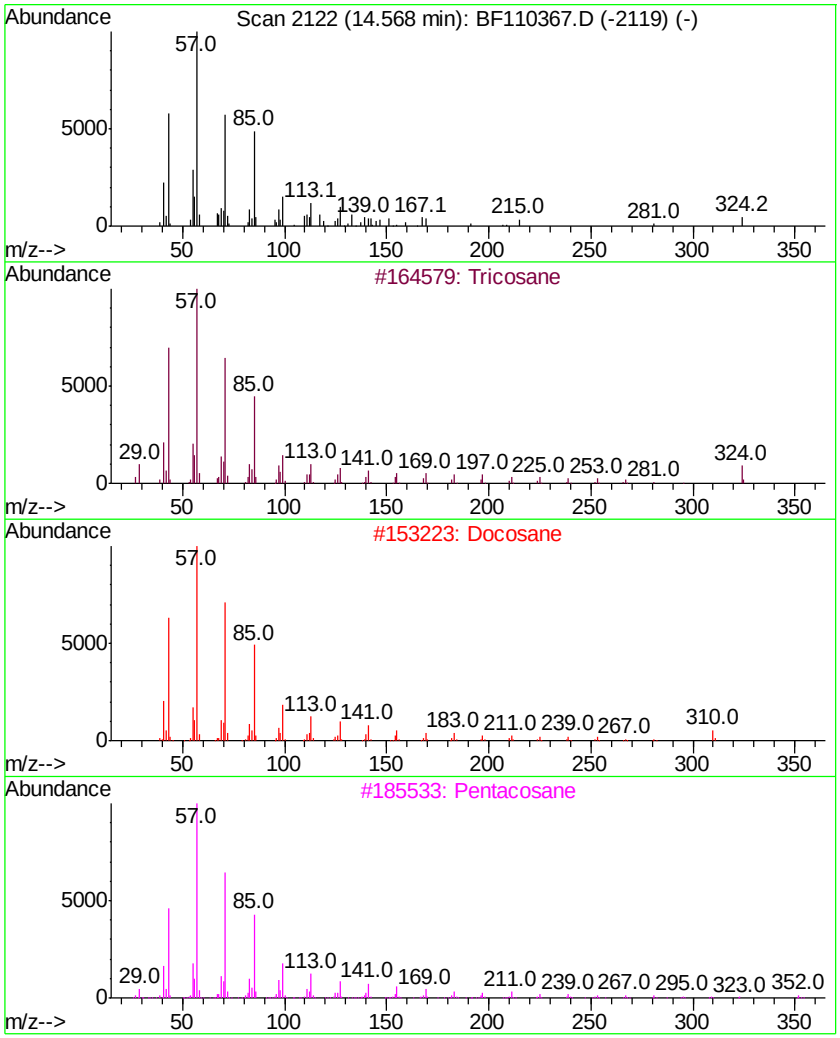
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

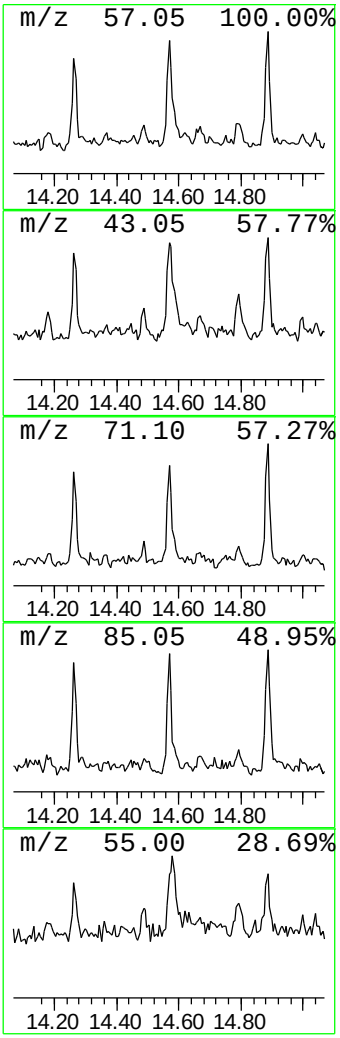
****

Peak Number 8 Tricosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.10 ng	70388	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	91
2	Docosane	310	C22H46	000629-97-0	87
3	Pentacosane	352	C25H52	000629-99-2	87
4	Heneicosane	296	C21H44	000629-94-7	74
5	Hexadecane, 8-hexyl-8-pentyl-	380	C27H56	055282-29-6	72





Library Search Compound Report

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
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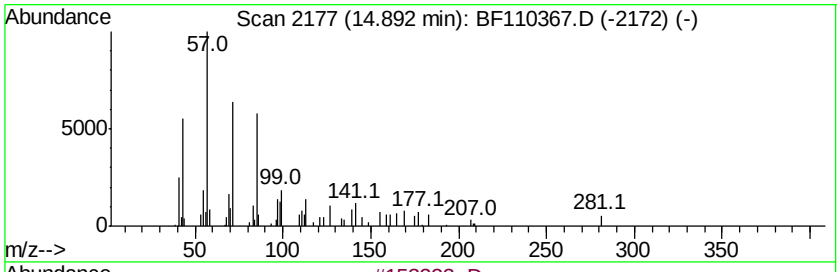
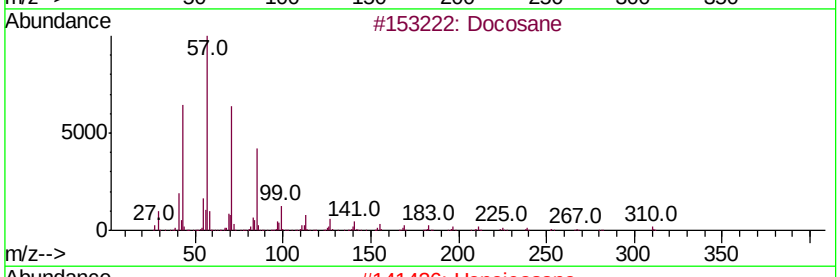
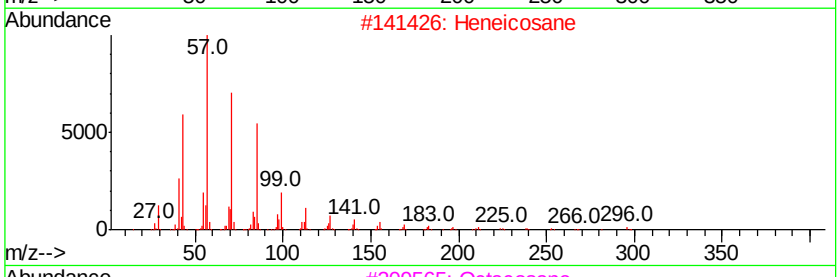
Peak Number 9 Docosane Concentration Rank 11

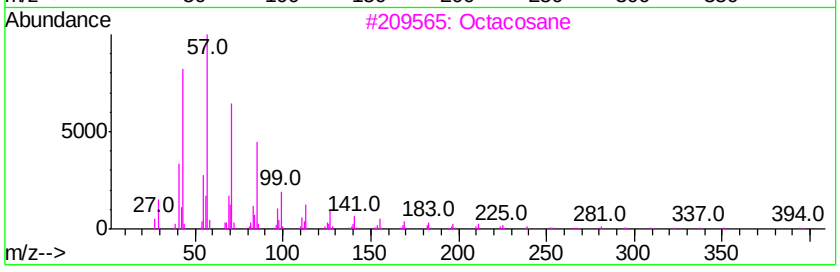
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.32 ng	52676	Chrysene-d12	14.13

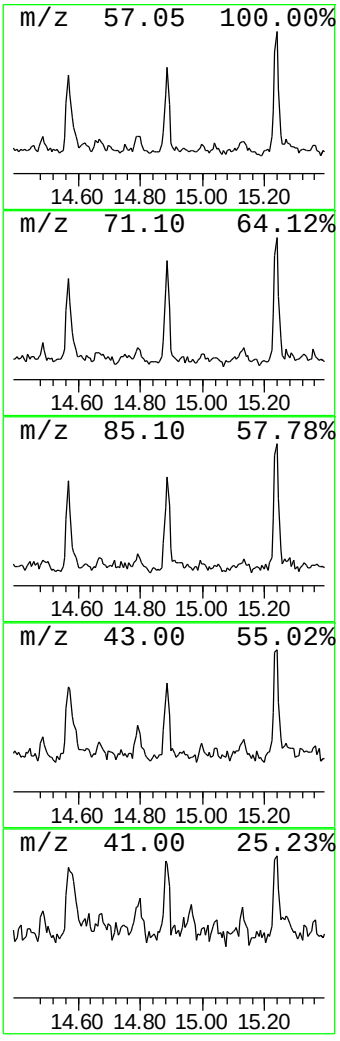
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Heneicosane	296	C21H44	000629-94-7	80
3	Octacosane	394	C28H58	000630-02-4	80
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	80
5	Tetracosane	338	C24H50	000646-31-1	80











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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

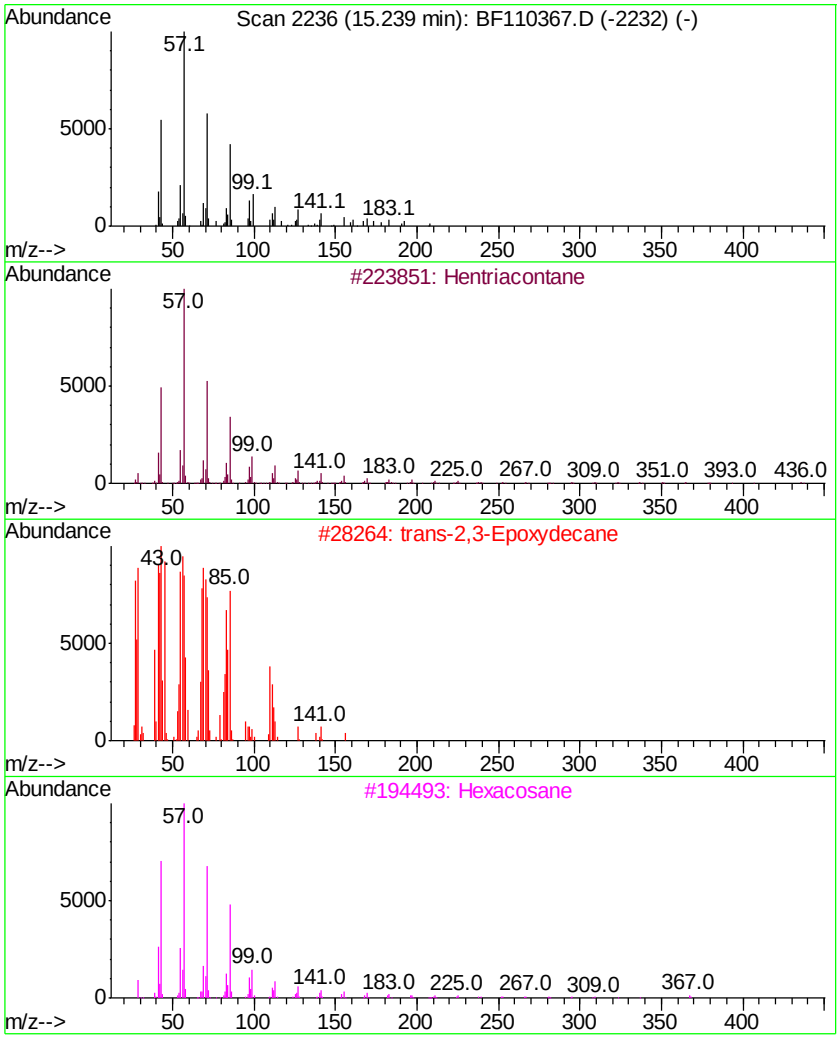
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

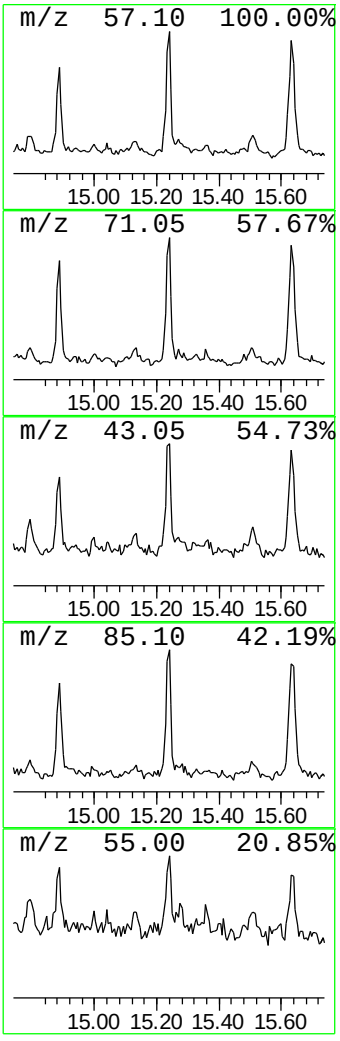
****

Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.71 ng	75102	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	86
5	Triacontane	422	C30H62	000638-68-6	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110118\
Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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

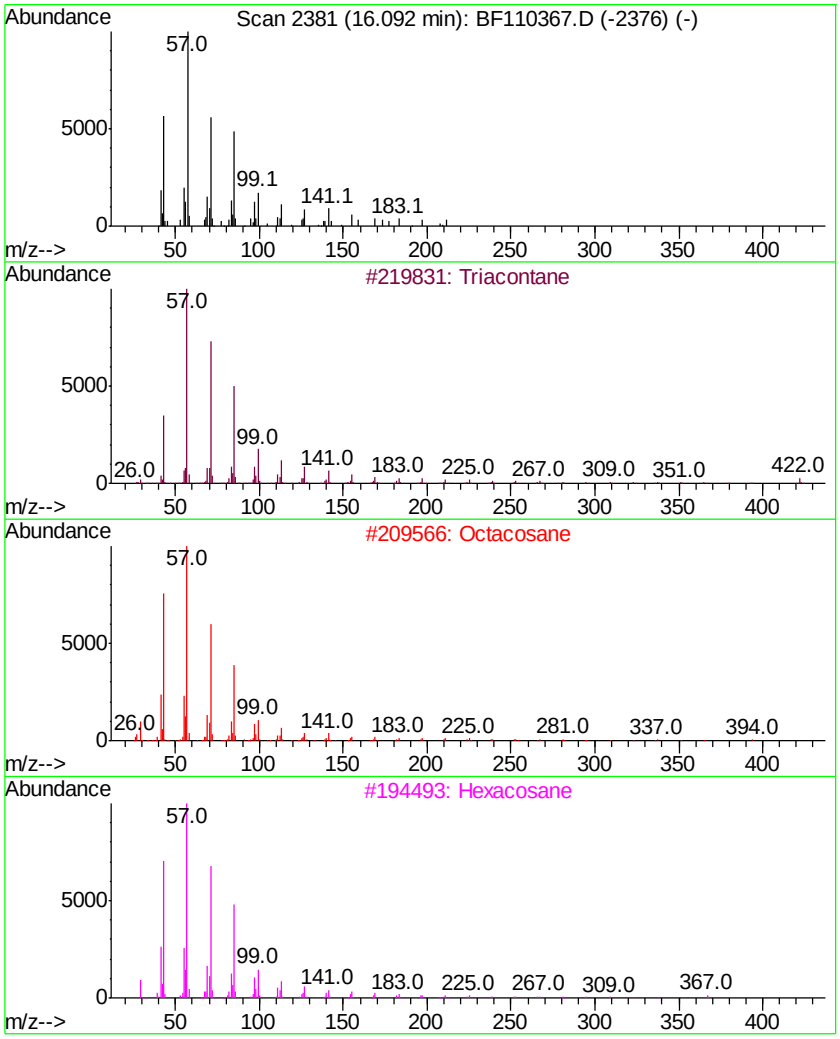
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

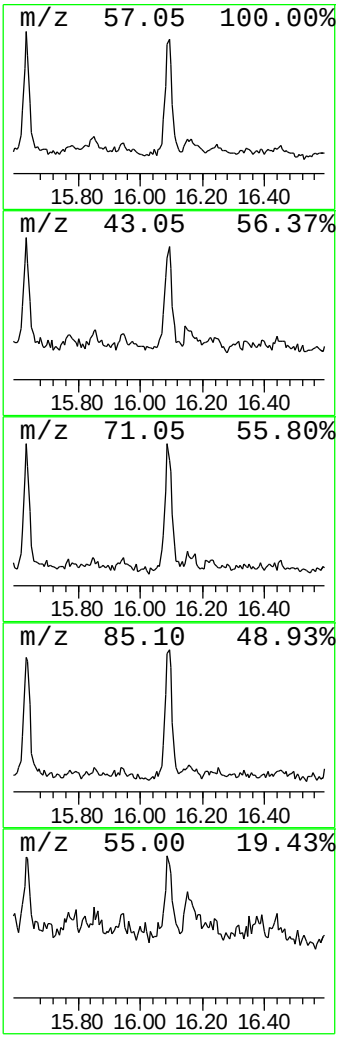
****

Peak Number 11 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	3.25 ng	89928	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Pentacosane	352	C25H52	000629-99-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110118\
Data File : BF110367.D
Acq On : 1 Nov 2018 14:34
Operator : JU/SJ
Sample : J5741-43
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11

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...	2.31	23.9	ng	626929	1	6.96	523980	20.0
R-(-)-1,2-propane...	3.59	3.1	ng	81033	1	6.96	523980	20.0
2-Pentanone, 4-hy...	5.21	5.0	ng	131457	1	6.96	523980	20.0
unknown6.73	6.73	109.2	ng	2860070	1	6.96	523980	20.0
Heptadecyl heptaf...	13.94	7.1	ng	160921	5	14.13	453529	20.0
2-Bromotetradecane	14.26	2.4	ng	54493	5	14.13	453529	20.0
Tricosane	14.57	3.1	ng	70388	5	14.13	453529	20.0
Docosane	14.89	2.3	ng	52676	5	14.13	453529	20.0
Hentriacontane	15.24	2.7	ng	75102	6	15.66	553737	20.0
Triacontane	16.09	3.3	ng	89928	6	15.66	553737	20.0