LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

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-BF100818.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	4.910	477	480	494	rBV	47140	79453	3.11%	0.364%
2	5.322	546	550	585	rBV	1603548	2208516	86.46%	10.116%
3	6.351	721	725	741	rBV	1781058	2474615	96.87%	11.335%
4	6.469	741	745	770	rVB	1969768	2540709	99.46%	11.638%
5	6.698	780	784	806	rVV	436399	648326	25.38%	2.970%
6	6.851	806	810	842	rVB	1775543	1906548	74.64%	8.733%
7	7.263	876	880	912	rBV	1186228	1587857	62.16%	7.273%
8	7.975	998	1001	1021	rBV	606348	764296	29.92%	3.501%
9	9.051	1180	1184	1198	rBV	2584301	2554464	100.00%	11.701%
10	9.445	1247	1251	1269	rBV	155480	177998	6.97%	0.815%
11	9.722	1294	1298	1321	rBV	719630	743668	29.11%	3.406%
12	10.386	1405	1411	1428	rBV4	15383	46494	1.82%	0.213%
13	10.510	1428	1432	1442	rBV	1150971	1267006	49.60%	5.804%
14	10.592	1442	1446	1452	rBV2	34423	80210	3.14%	0.367%
15	11.198	1546	1549	1562	rBV	532075	639858	25.05%	2.931%
16	11.739	1638	1641	1650	rBV2	44439	64153	2.51%	0.294%
17	12.410	1751	1755	1765	rBV	47943	58966	2.31%	0.270%
18	12.633	1789	1793	1797	rVB	45403	43257	1.69%	0.198%
19	12.780	1814	1818	1828	rBV	2004192	1855405	72.63%	8.499%
20	13.263	1894	1900	1906	rBV	125486	141855	5.55%	0.650%
21	13.686	1969	1972	1984	rBV4	84450	156677	6.13%	0.718%
22	13.827	1987	1996	2009	rBV	589281	728366	28.51%	3.336%
23	14.298	2073	2076	2080	rVB	36565	34617	1.36%	0.159%
24	14.592	2123	2126	2131	rVB	55771	50575	1.98%	0.232%
25	14.833	2163	2167	2175	rBV	45293	89718	3.51%	0.411%
26	14.904	2175	2179	2183	rBV	69422	76809	3.01%	0.352%
27	15.110	2210	2214	2219	rBV	23021	28372	1.11%	0.130%
28	15.168	2221	2224	2228	rVB	20932	26243	1.03%	0.120%
29	15.221	2228	2233	2237	rBV	392298	512709	20.07%	2.348%
30	15.645	2300	2305	2311	rBV	80527	114962	4.50%	0.527%
31	16.104	2378	2383	2393	rVB2	38335	76583	3.00%	0.351%
32	16.639	2469	2474	2483	rVB2	27488	52390	2.05%	0.240%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

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-BF100818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 21831675

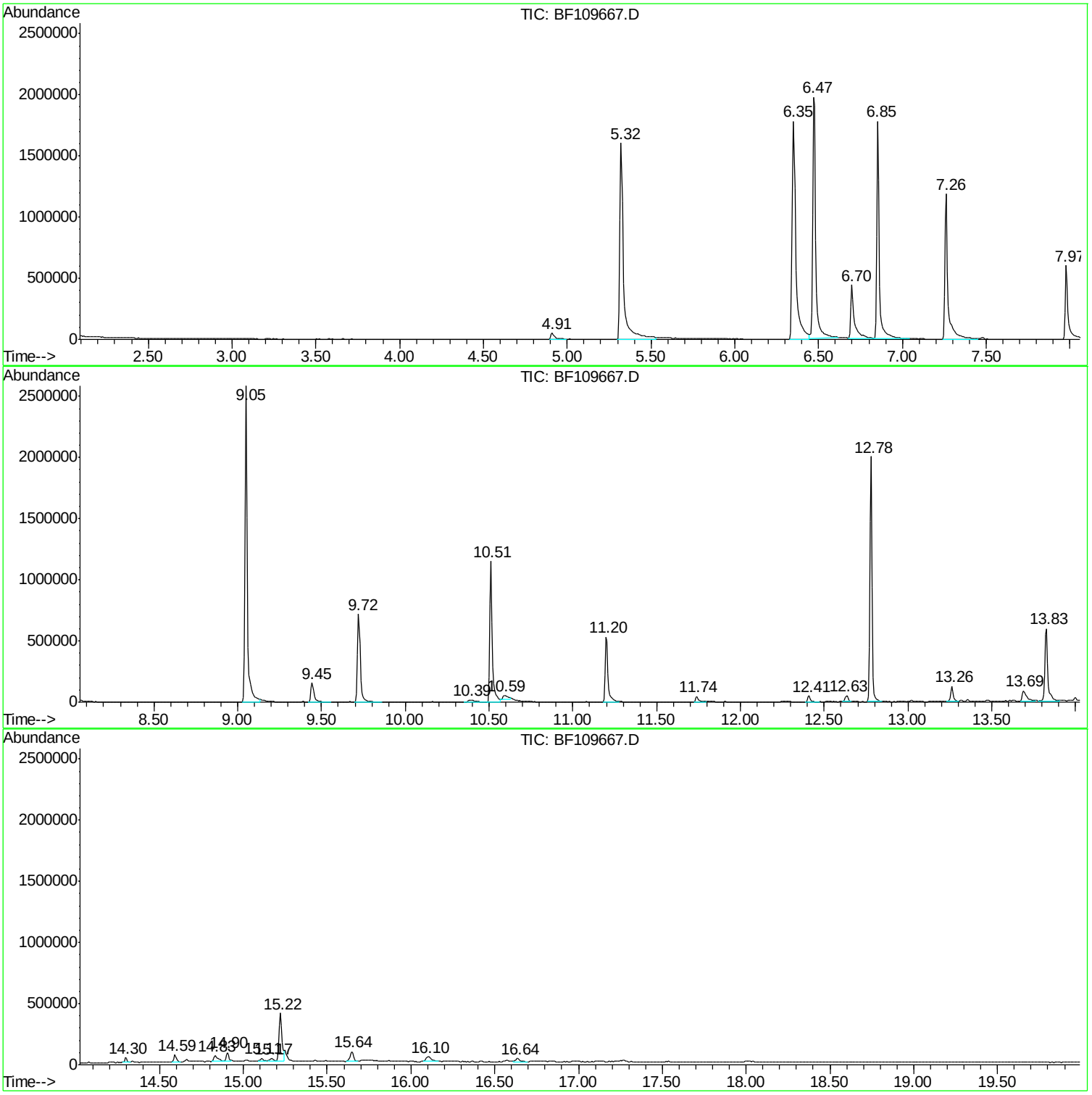
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

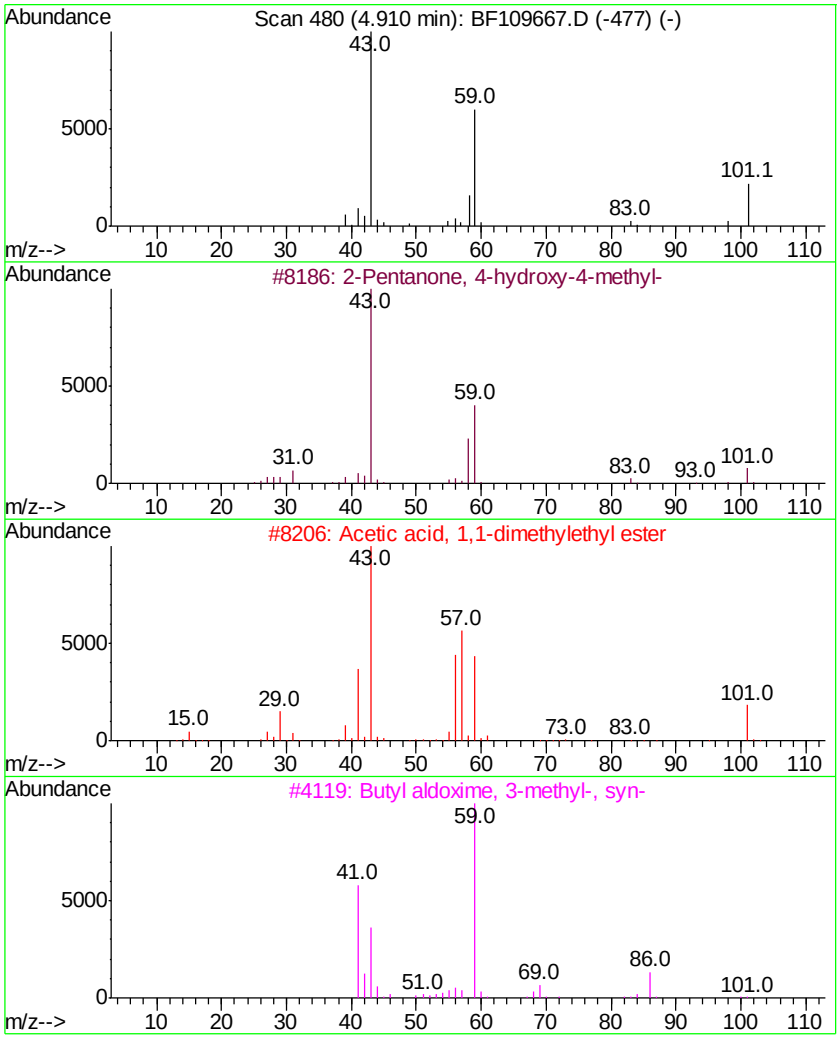
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

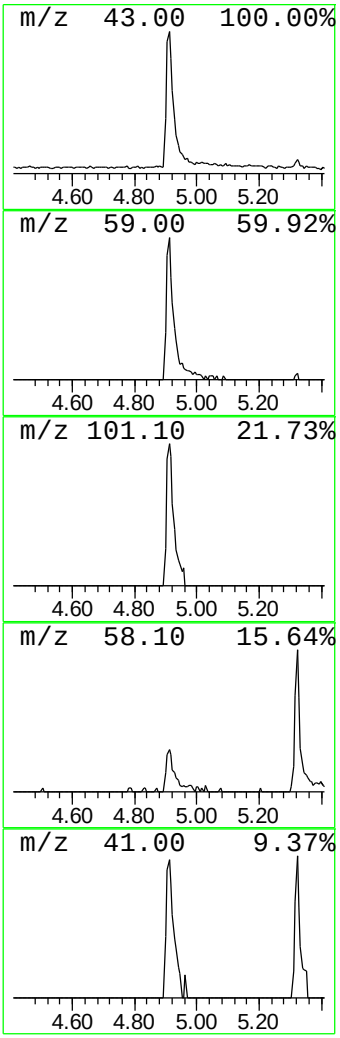
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.45 ng	79453	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

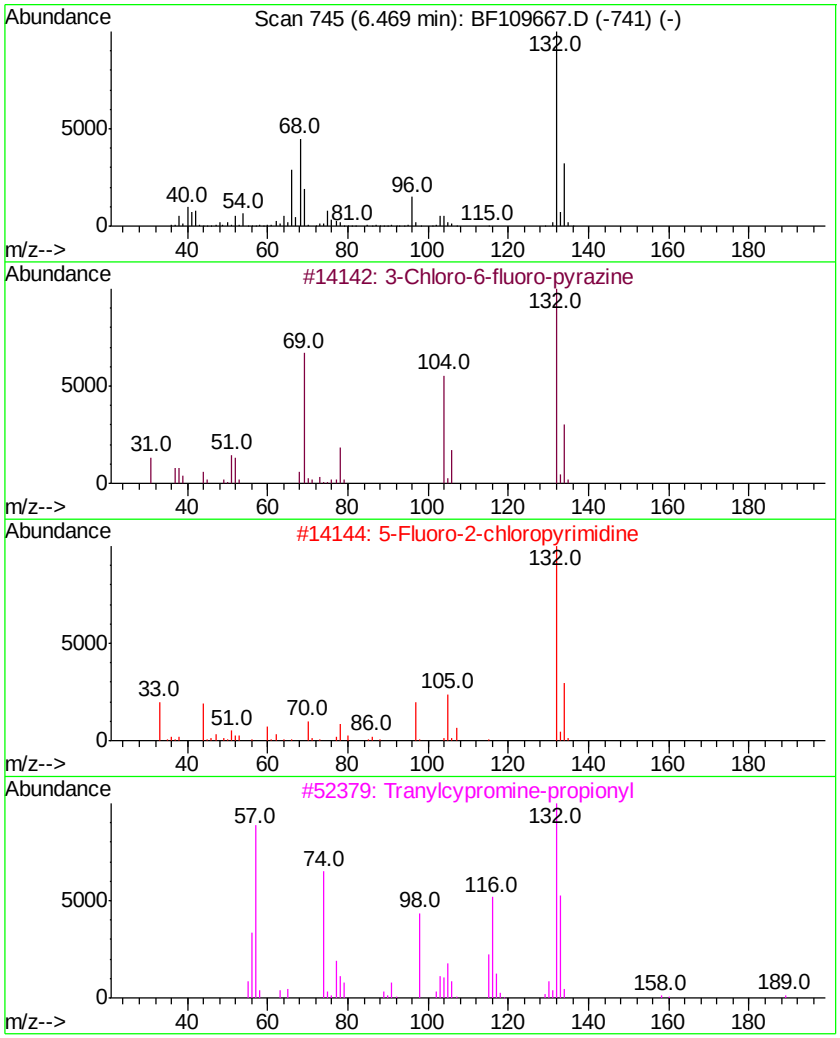
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

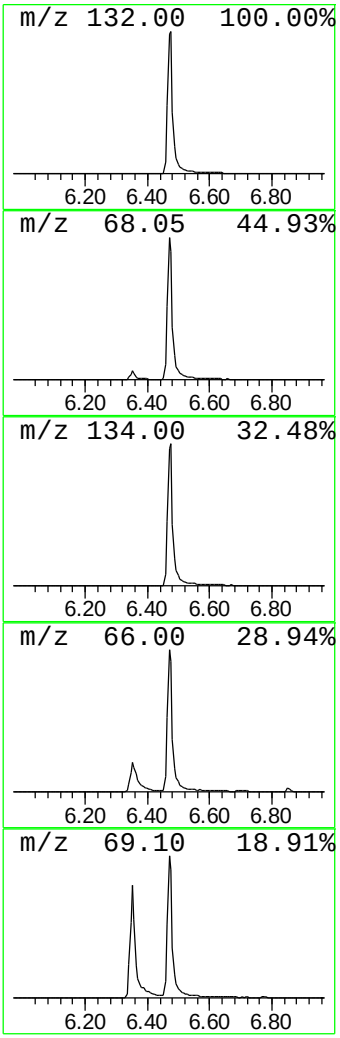
****

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	78.38 ng	2540710	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

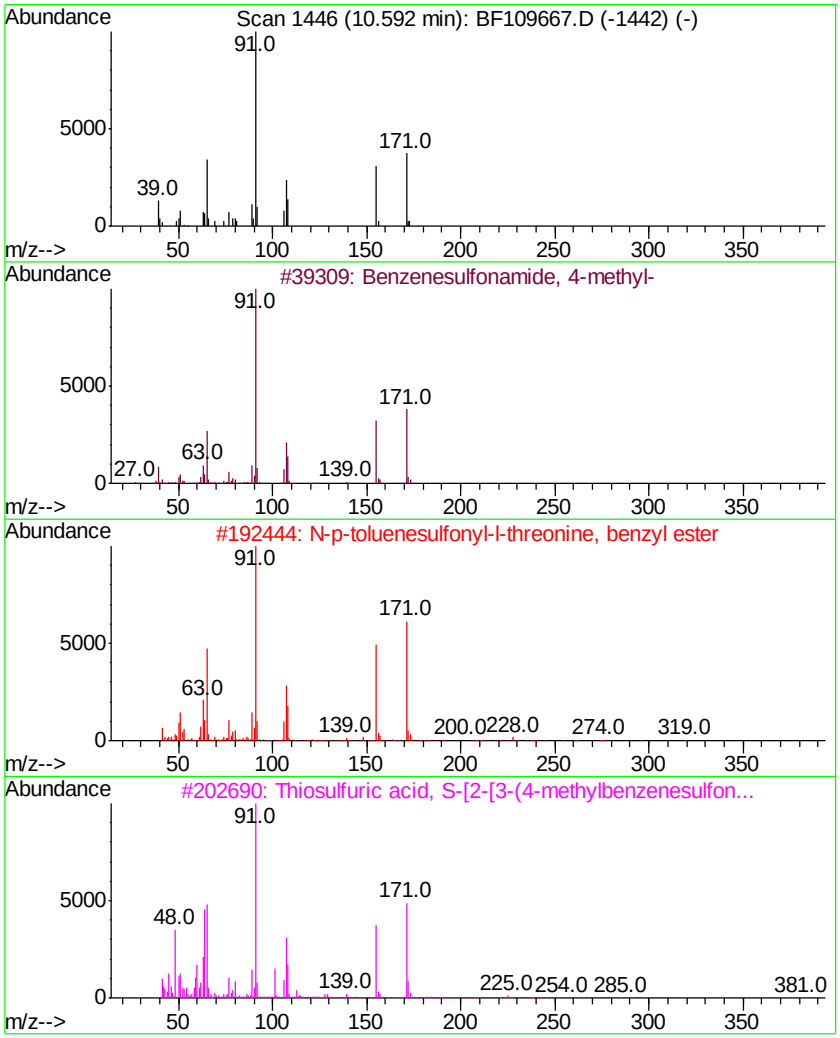
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

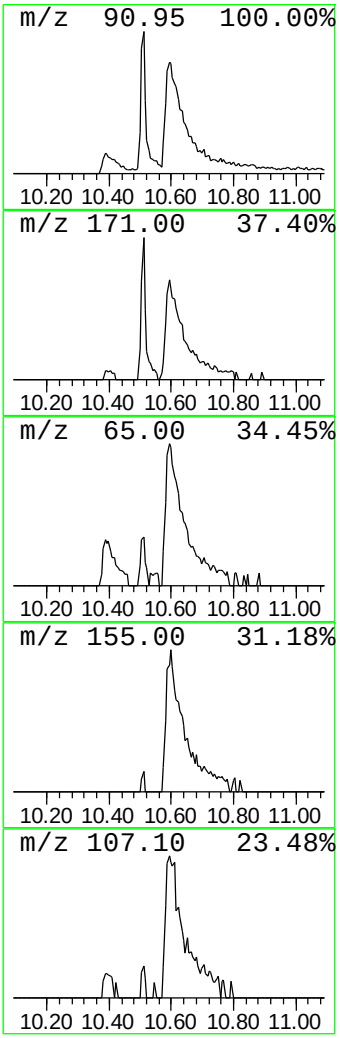
****

Peak Number 4 Benzenesulfonamide, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	2.51 ng	80210	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	96
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	87
3	Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	83
4	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	59
5	Thiophene-3-ol, 2,3-dihydro-, 4-...	288	C11H12O5S2	039582-96-2	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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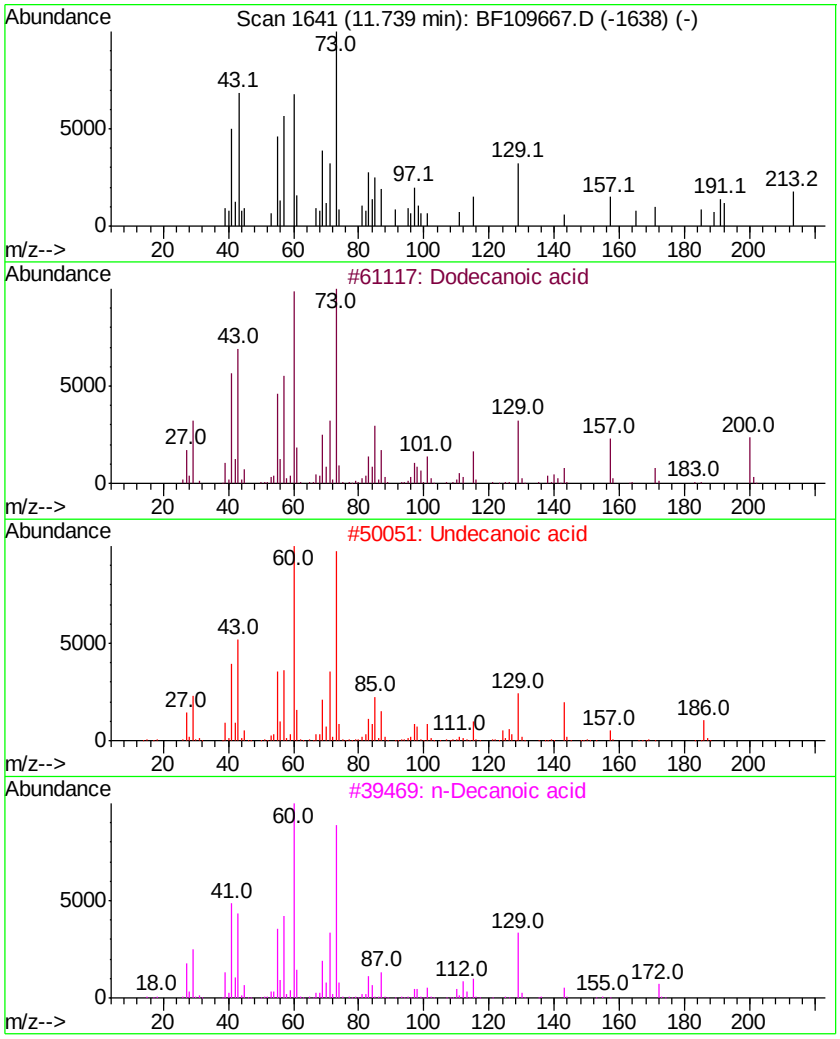
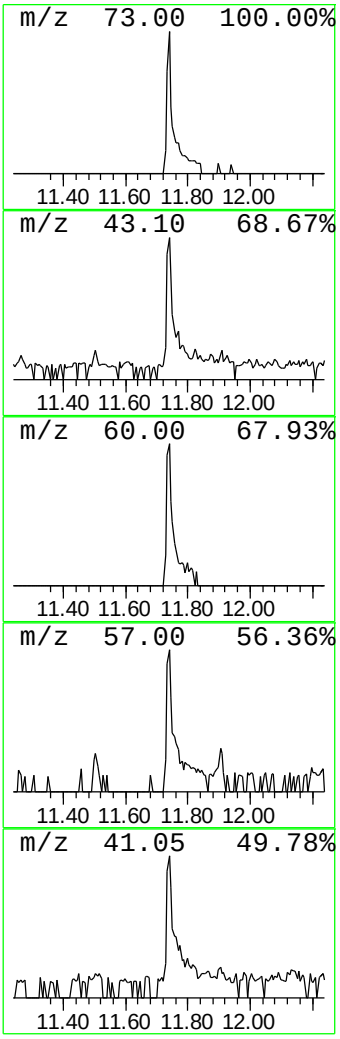
****

Peak Number 5 Dodecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.01 ng	64153	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	53
2	Undecanoic acid	186	C11H22O2	000112-37-8	40
3	n-Decanoic acid	172	C10H20O2	000334-48-5	38
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	35
5	Nonanoic acid	158	C9H18O2	000112-05-0	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

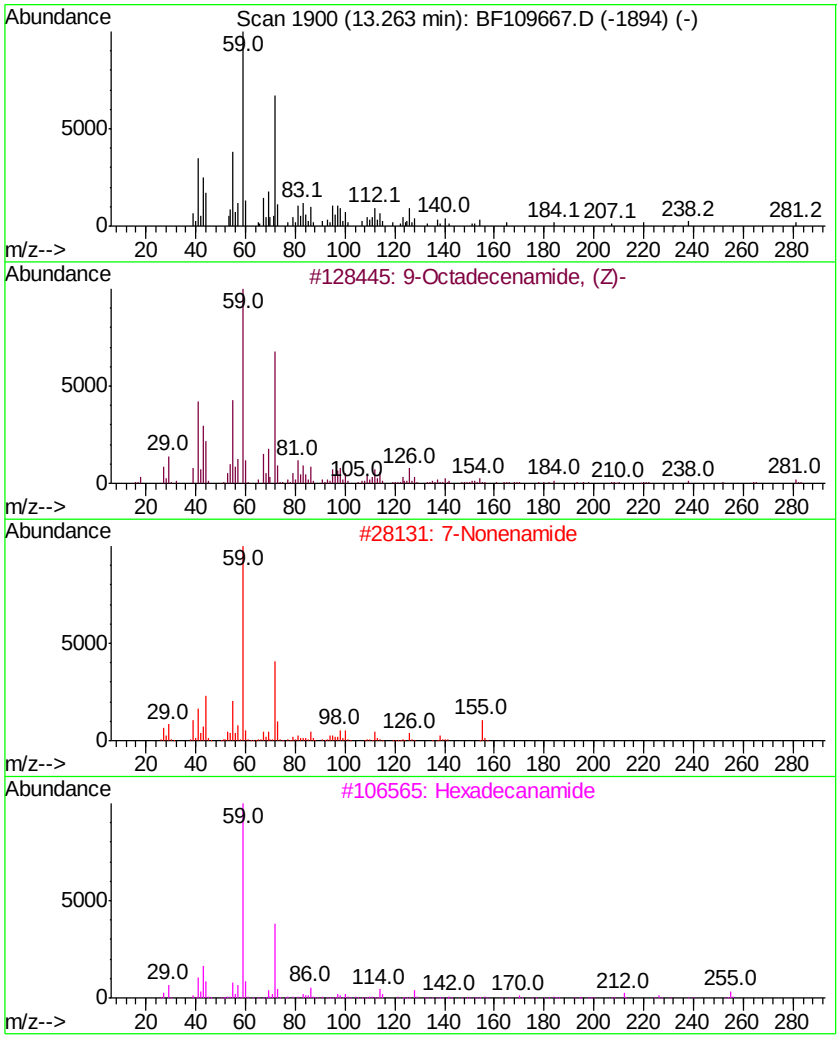
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

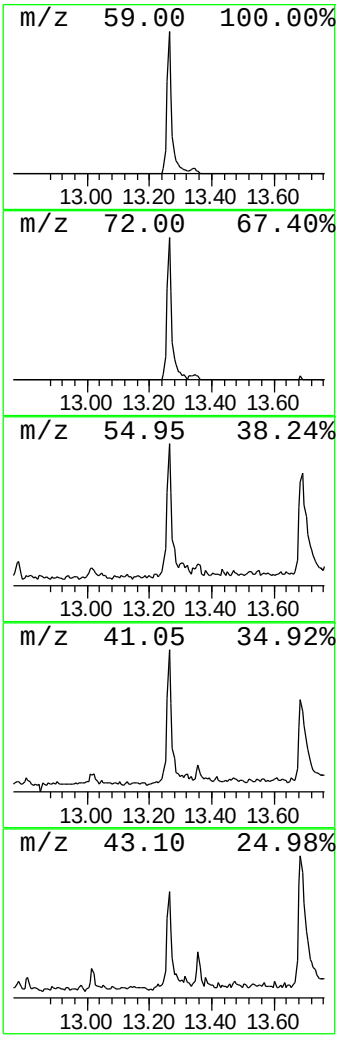
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	3.90 ng	141855	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	7-Nonenamide	155	C9H17NO	090949-53-4	72
3	Hexadecanamide	255	C16H33NO	000629-54-9	59
4	Tetradecanamide	227	C14H29NO	000638-58-4	50
5	Dodecanamide	199	C12H25NO	001120-16-7	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

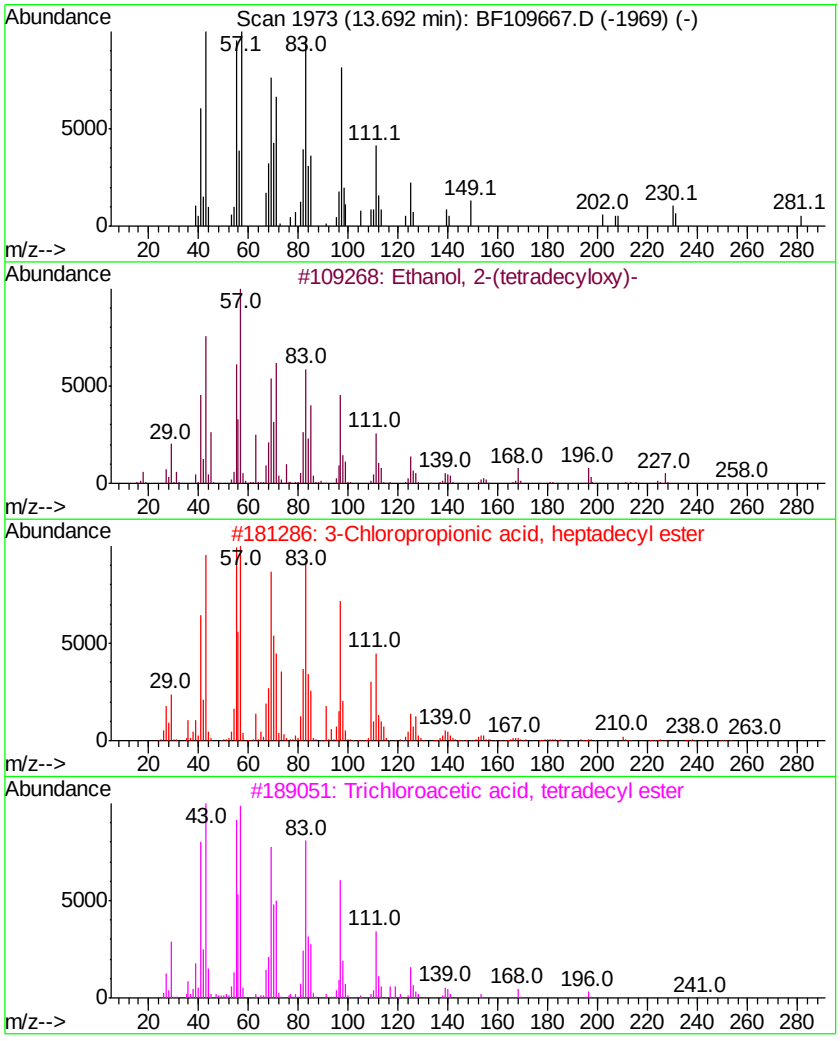
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

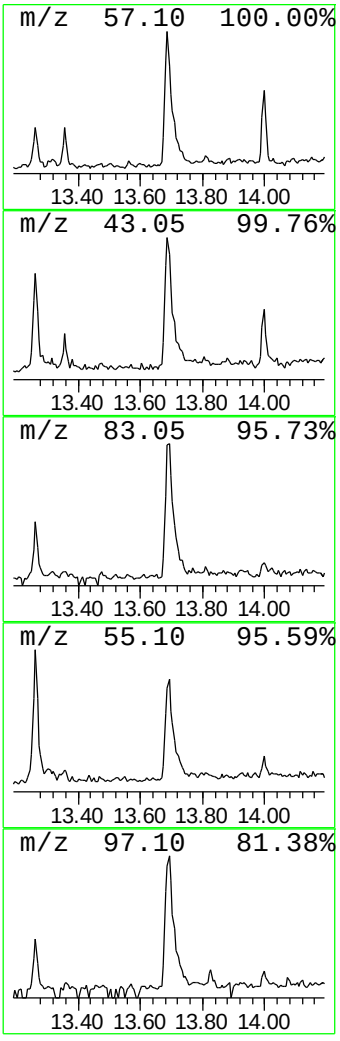
****

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	4.30 ng	156677	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	81
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	81
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	81
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

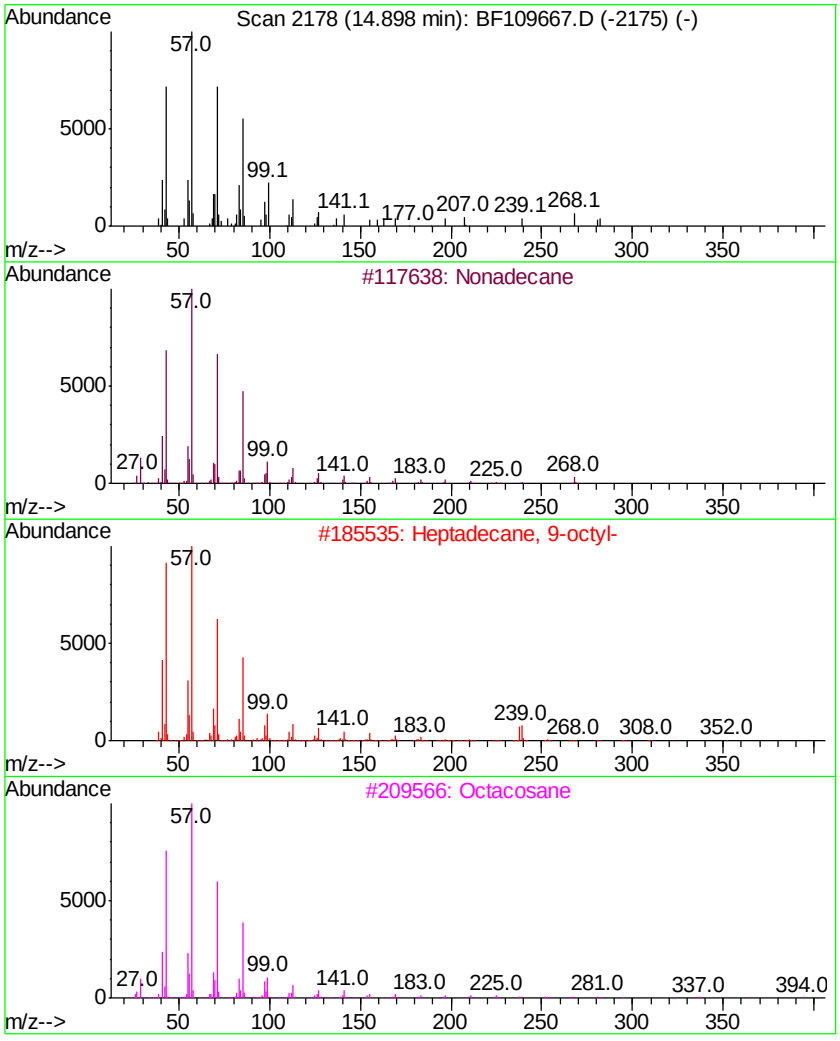
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

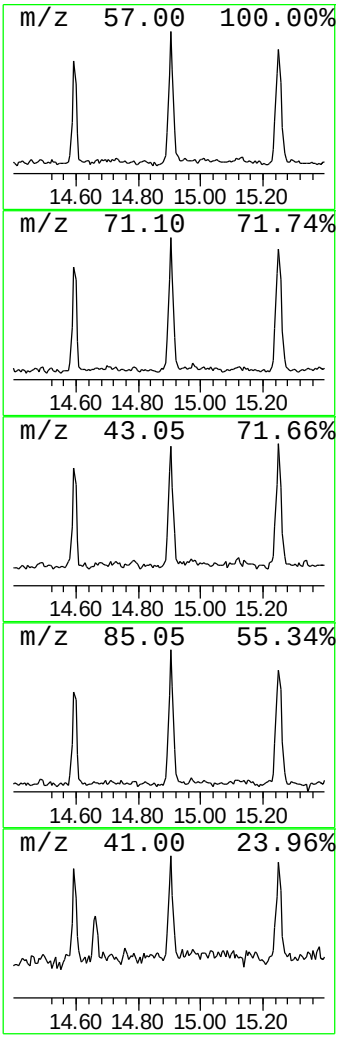
****

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	3.00 ng	76809	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Triacontane	422	C30H62	000638-68-6	91





Library Search Compound Report

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Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

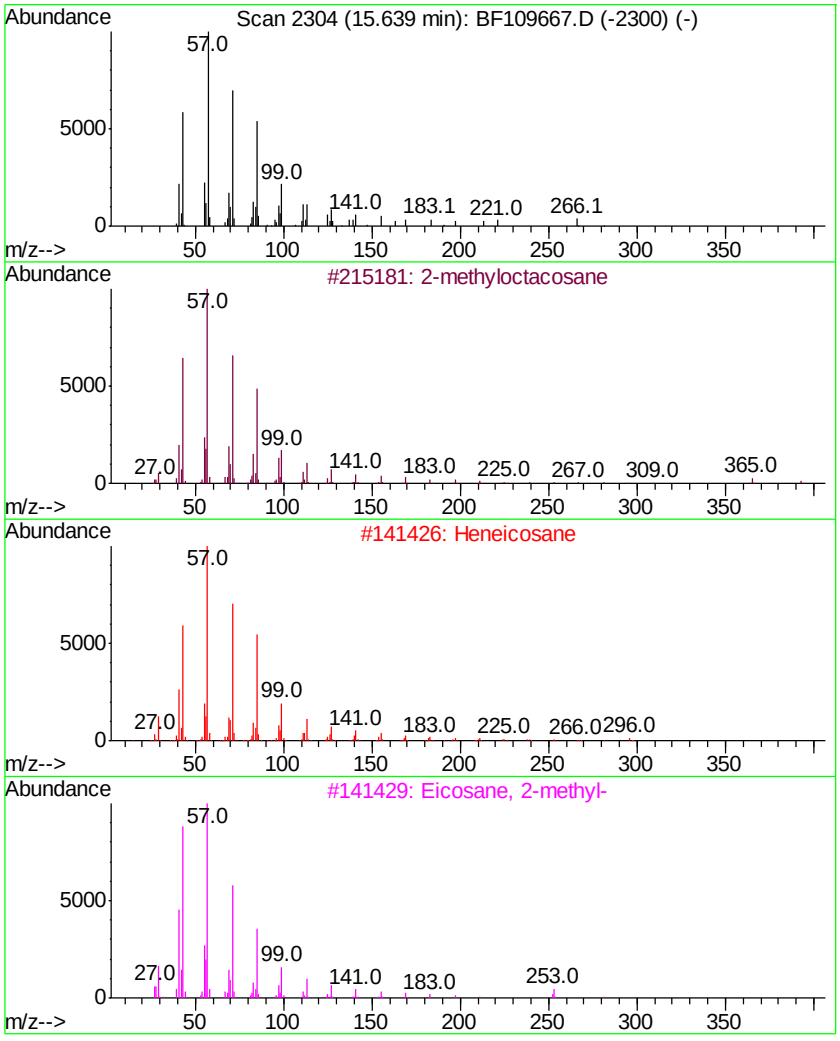
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

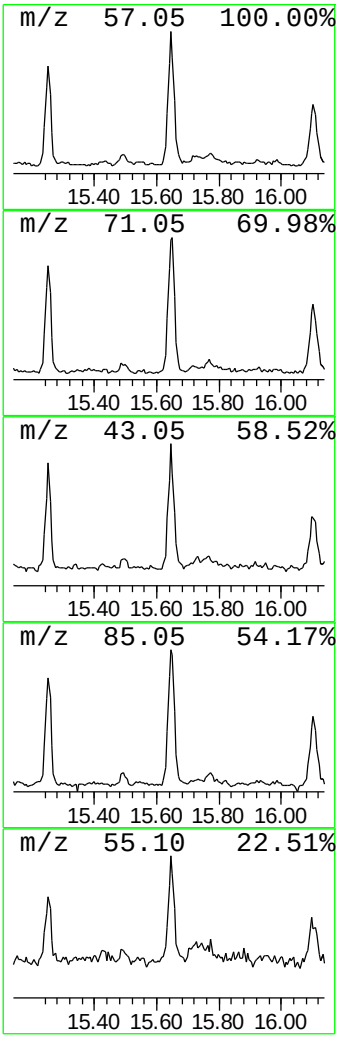
****

Peak Number 9 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	4.48 ng	114962	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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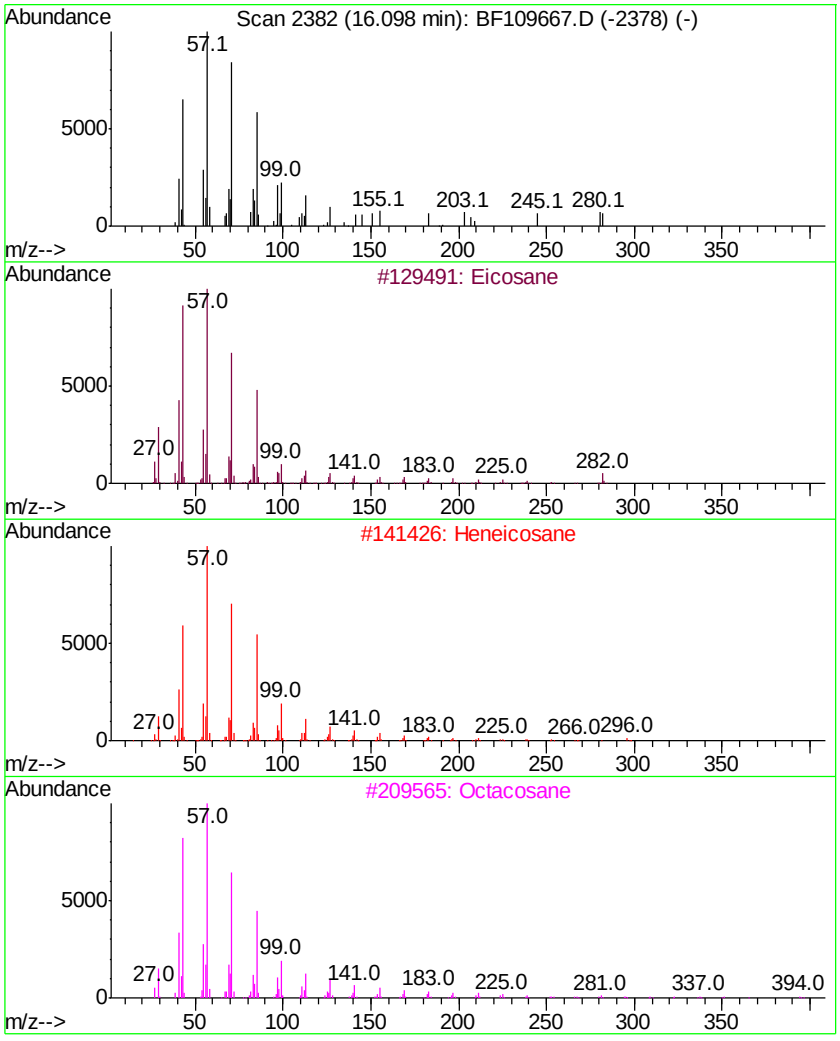
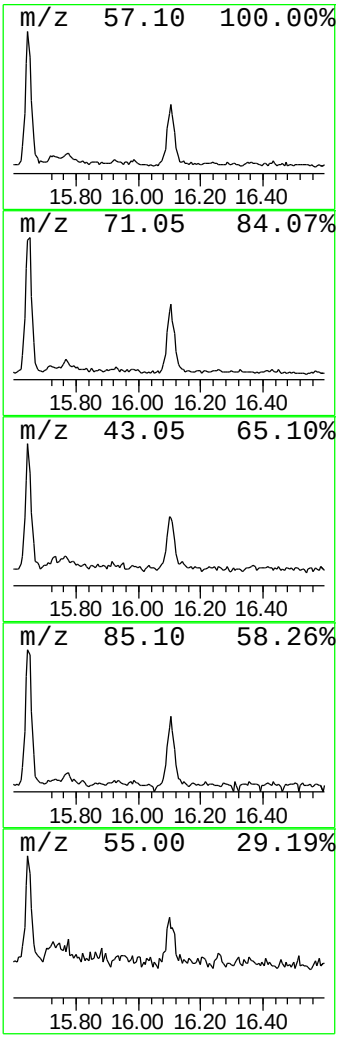
Peak Number 10 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.99 ng	76583	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Pentacosane	352	C25H52	000629-99-2	87





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Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

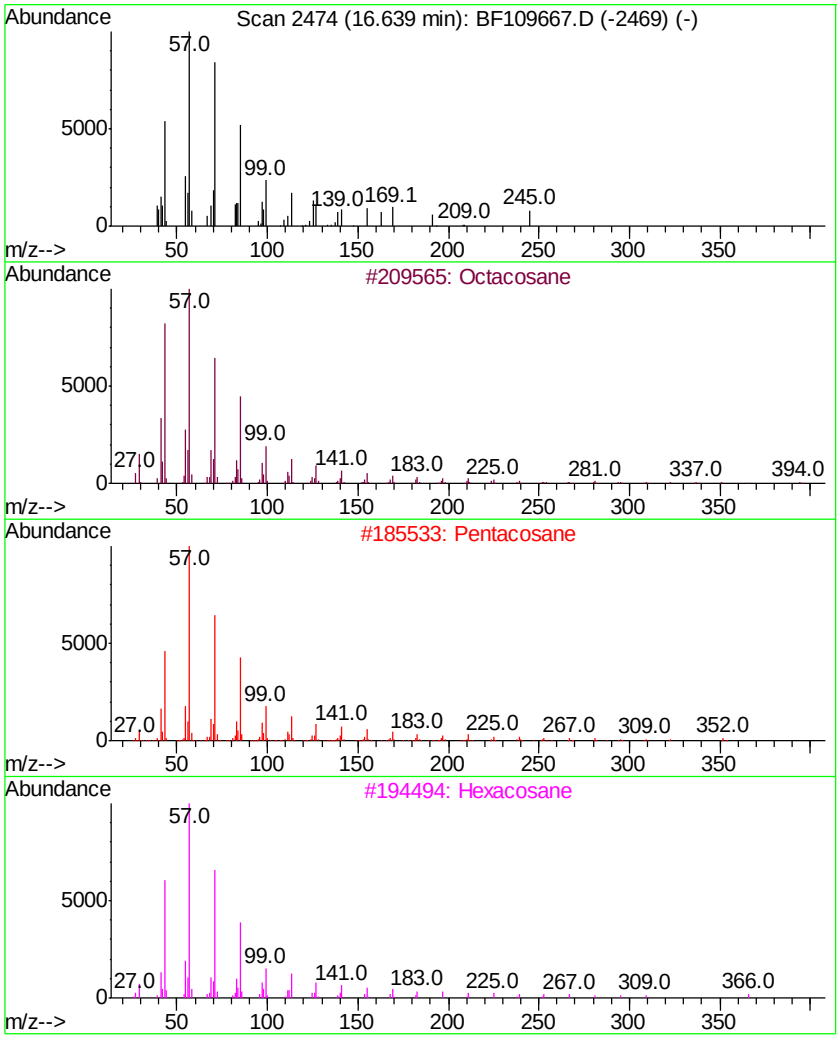
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

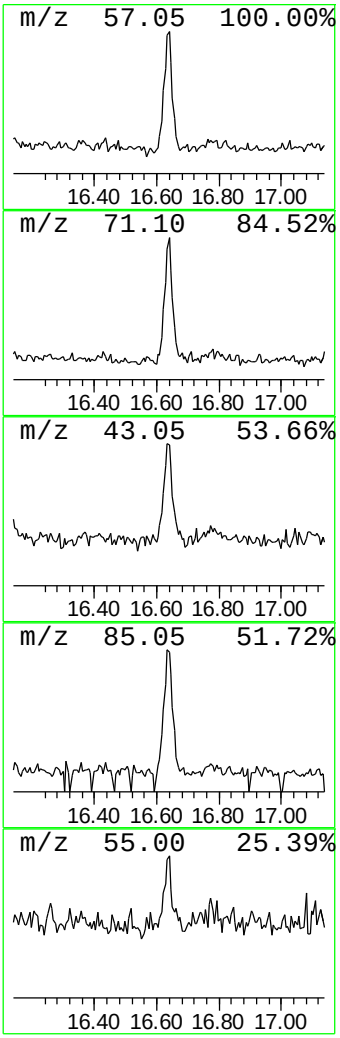
****

Peak Number 11 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	2.04 ng	52390	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Pentacosane	352	C25H52	000629-99-2	86
3	Hexacosane	366	C26H54	000630-01-3	86
4	Triacontane	422	C30H62	000638-68-6	86
5	Tetracosane	338	C24H50	000646-31-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100818\
Data File : BF109667.D
Acq On : 9 Oct 2018 00:17
Operator : JU/SJ
Sample : J5287-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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
2-Pentanone, 4-hy...	4.91	2.5	ng	79453	1	6.70	648326	20.0
unknown6.47	6.47	78.4	ng	2540710	1	6.70	648326	20.0
Benzenesulfonamid...	10.59	2.5	ng	80210	4	11.20	639858	20.0
Dodecanoic acid	11.74	2.0	ng	64153	4	11.20	639858	20.0
9-Octadecenamide,...	13.26	3.9	ng	141855	5	13.83	728366	20.0
Ethanol, 2-(tetra...	13.69	4.3	ng	156677	5	13.83	728366	20.0
Nonadecane	14.90	3.0	ng	76809	6	15.22	512709	20.0
2-methyloctacosane	15.64	4.5	ng	114962	6	15.22	512709	20.0
Eicosane	16.10	3.0	ng	76583	6	15.22	512709	20.0
Octacosane	16.64	2.0	ng	52390	6	15.22	512709	20.0