LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118597.D
Acq On : 20 Jan 2020 18:04
Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

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-BF012020.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	2.193	11	18	24	rBV	1919872	2516043	20.09%	2.185%
2	5.098	504	512	523	rBV	1534691	1894041	15.12%	1.645%
3	5.498	575	580	583	rBV	8109102	8254525	65.90%	7.168%
4	6.504	744	751	754	rBV	8535144	8940506	71.38%	7.764%
5	6.645	770	775	779	rBV	8668171	9207869	73.51%	7.996%
6	6.881	811	815	818	rBV	3180774	2732964	21.82%	2.373%
7	7.039	837	842	845	rVB	7678911	7362134	58.78%	6.393%
8	7.434	904	909	912	rBV	5622843	5696110	45.48%	4.947%
9	8.163	1028	1033	1036	rBV	3811996	3539769	28.26%	3.074%
10	9.239	1210	1216	1219	rBV	12142384	11409321	91.09%	9.908%
11	9.628	1278	1282	1285	rBV	507142	414467	3.31%	0.360%
12	9.916	1325	1331	1335	rBV	5015875	4409317	35.20%	3.829%
13	10.704	1459	1465	1468	rBV	8309726	7687537	61.38%	6.676%
14	11.404	1579	1584	1587	rBV	5000886	4573784	36.52%	3.972%
15	11.927	1668	1673	1677	rBV	125826	149034	1.19%	0.129%
16	12.992	1849	1854	1857	rBV	11855204	12525454	100.00%	10.877%
17	13.880	2002	2005	2017	rBV	1893354	2087143	16.66%	1.812%
18	14.039	2027	2032	2035	rBV	3391941	3337206	26.64%	2.898%
19	14.210	2056	2061	2067	rBV	1067031	1061286	8.47%	0.922%
20	14.515	2107	2113	2126	rBV	2200366	2124453	16.96%	1.845%
21	14.827	2160	2166	2176	rBV	2580725	2959113	23.62%	2.570%
22	15.168	2218	2224	2233	rBV	2576381	3106751	24.80%	2.698%
23	15.504	2276	2281	2285	rBV	2138030	2793364	22.30%	2.426%
24	15.557	2285	2290	2308	rVB	1956692	2864147	22.87%	2.487%
25	15.998	2358	2365	2370	rBV	1210790	1975999	15.78%	1.716%
26	16.039	2370	2372	2382	rVB2	172415	272997	2.18%	0.237%
27	16.509	2446	2452	2467	rVB	511880	1016080	8.11%	0.882%
28	17.115	2550	2555	2562	rVB2	124024	241767	1.93%	0.210%

Sum of corrected areas: 115153181

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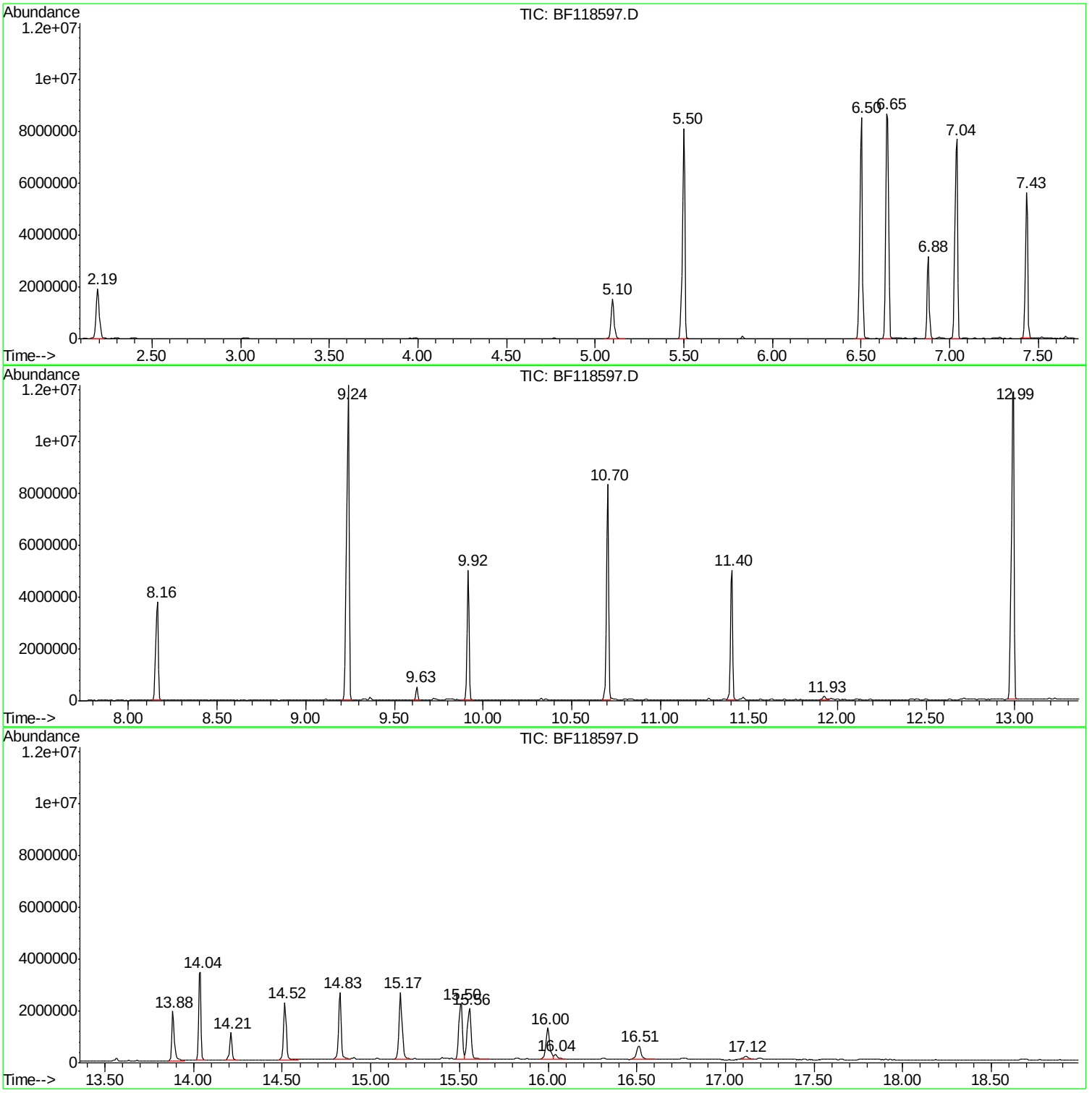
Instrument :
BNA_F
ClientSampleId :
PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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 : BF118597.D
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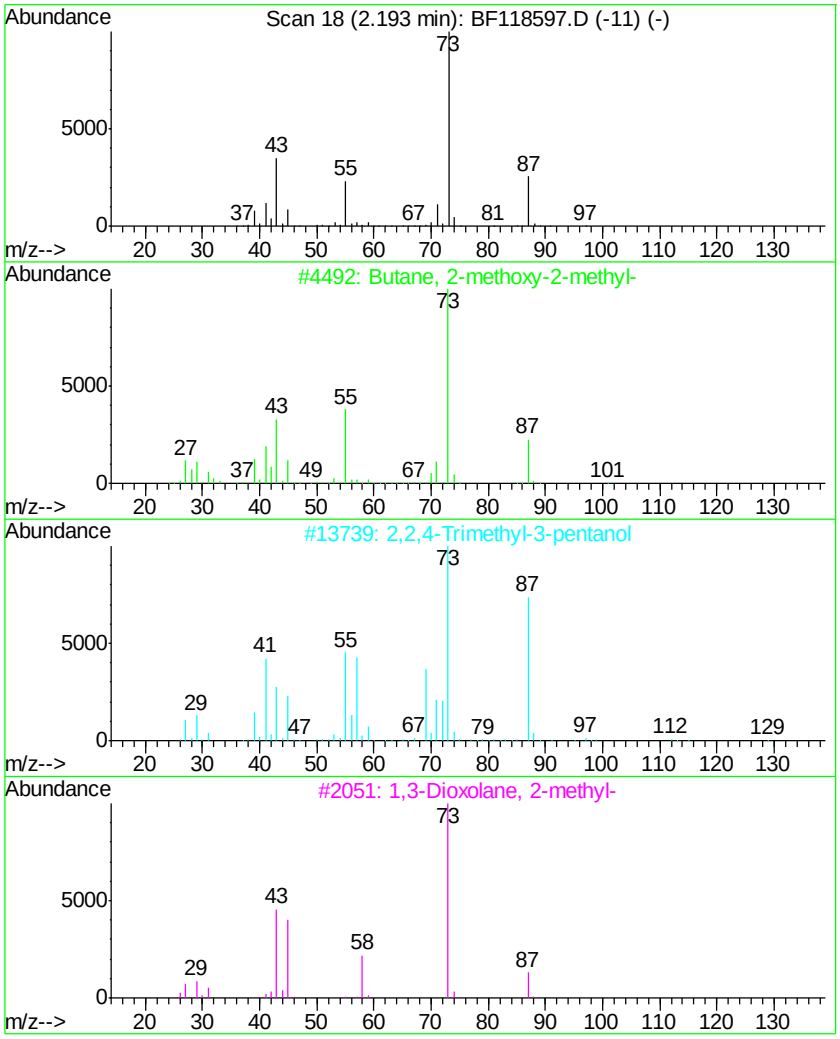
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

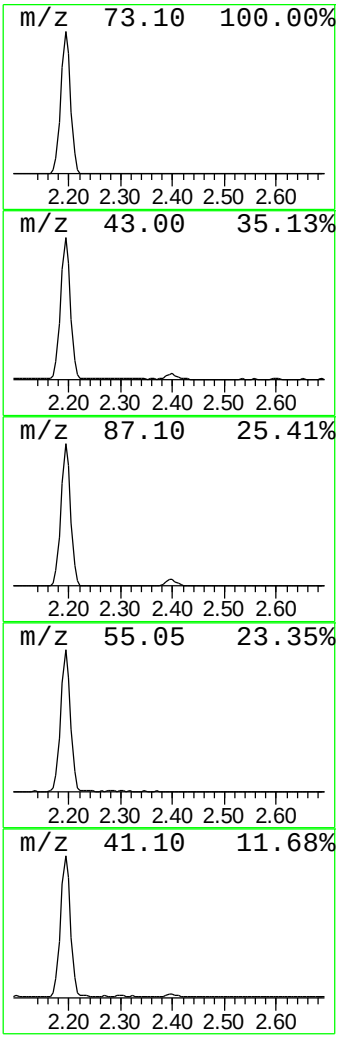
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	18.41 ng	2516040	1,4-Dichlorobenzene-d4	6.88

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	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

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Data File : BF118597.D
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Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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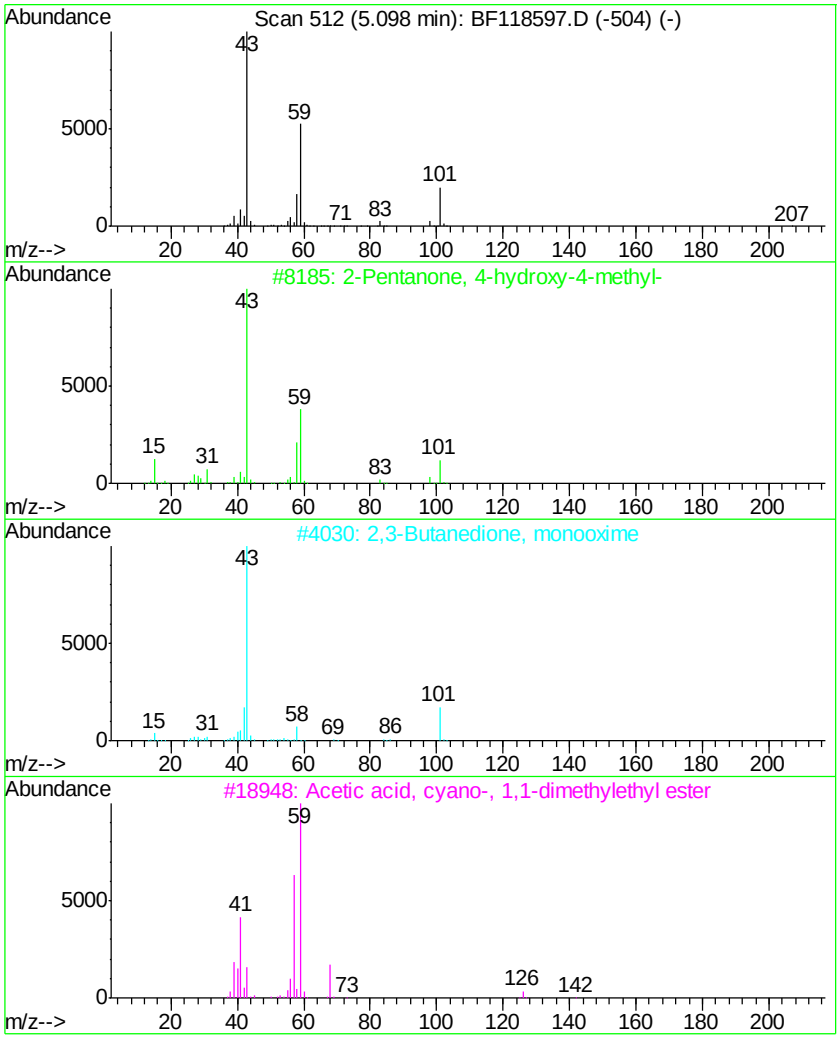
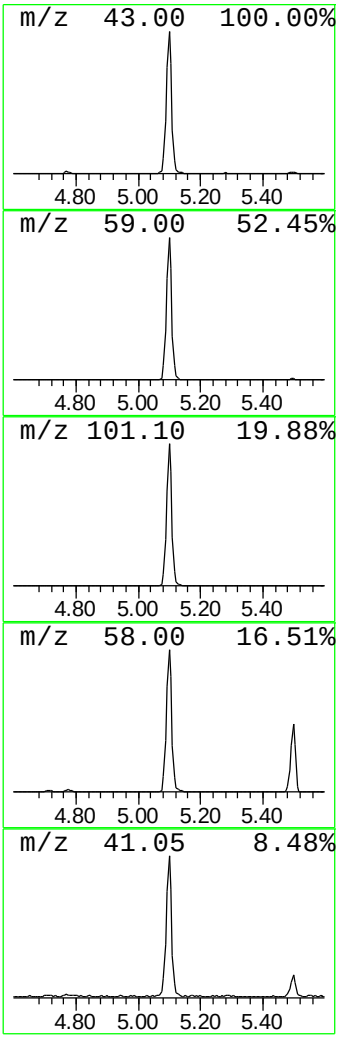
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	13.86 ng	1894040	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Acetone	58	C3H6O	000067-64-1	10
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

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Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

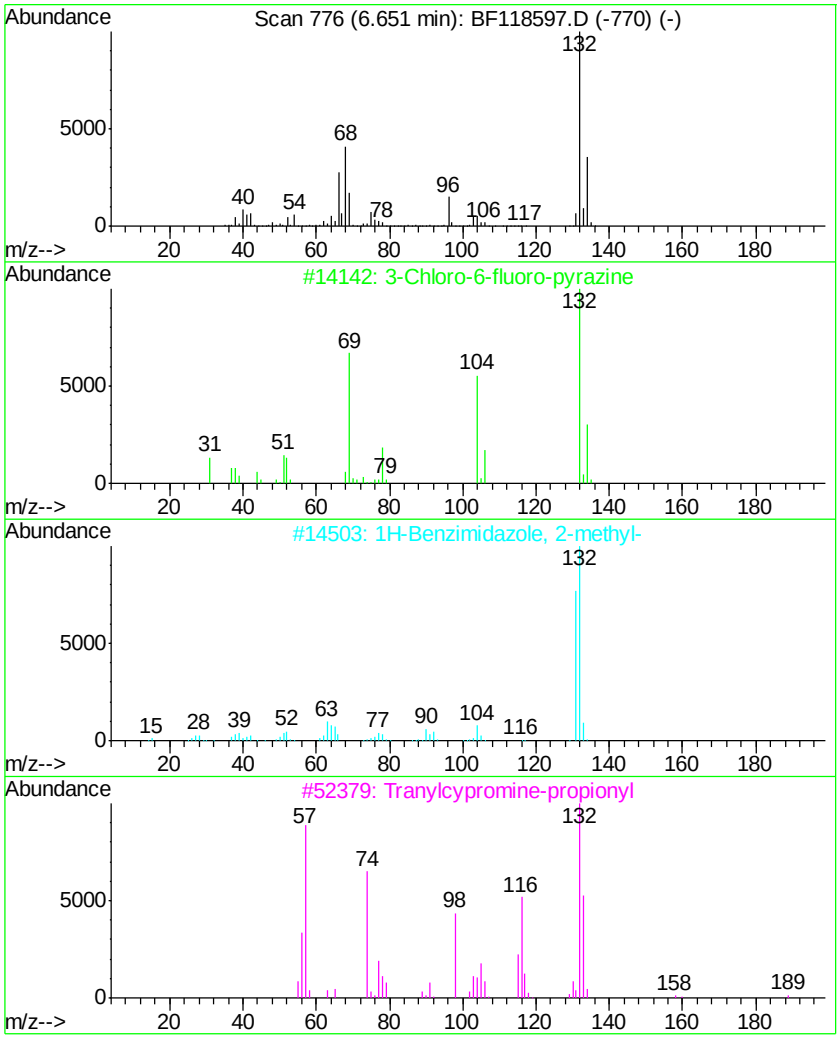
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

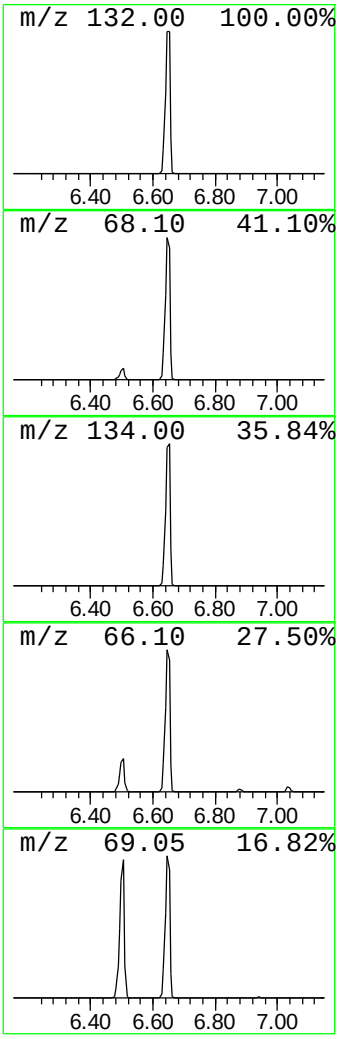
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	67.38 ng	9207870	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

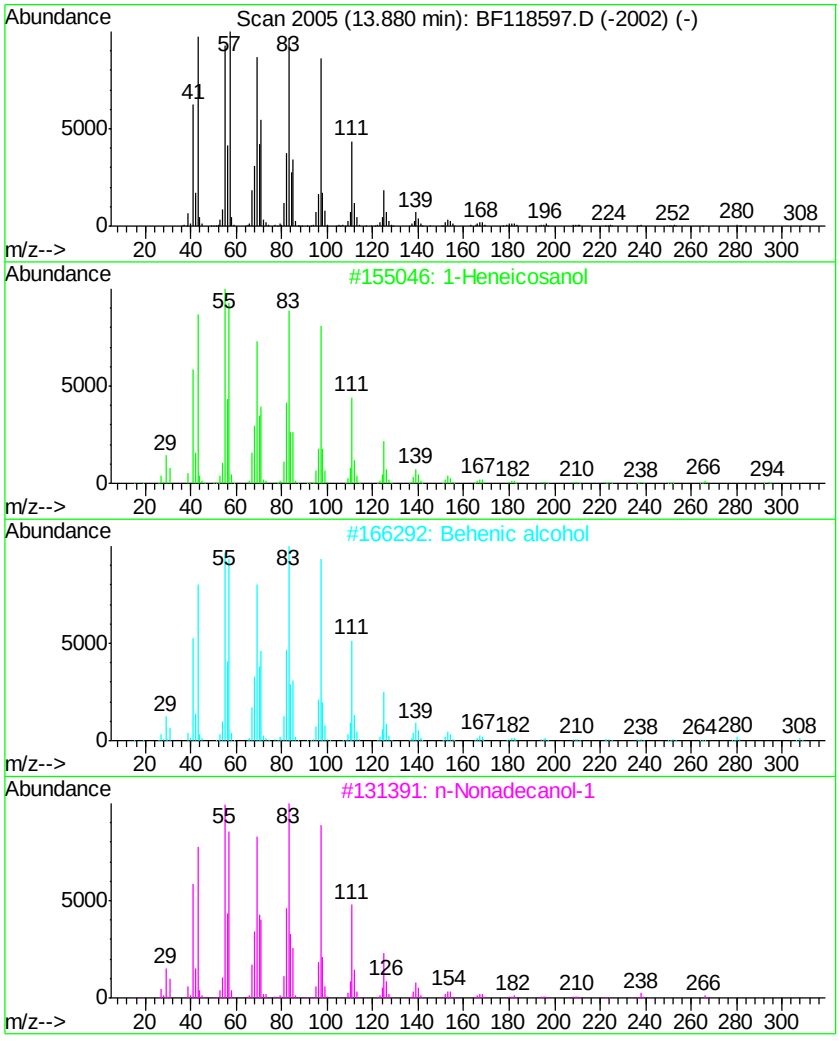
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

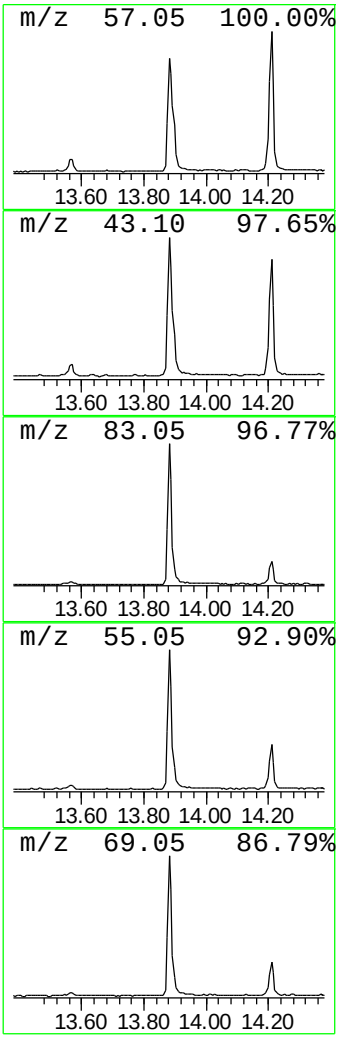
****

Peak Number 5 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	12.51 ng	2087140	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118597.D
Acq On : 20 Jan 2020 18:04
Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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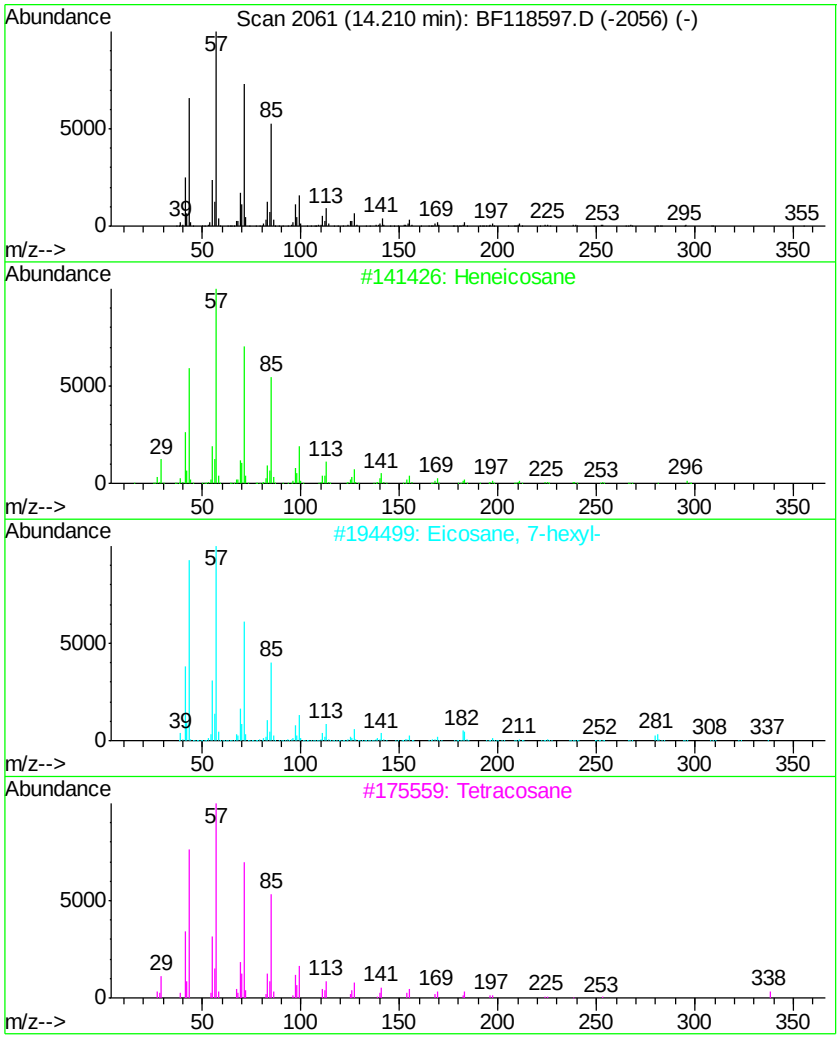
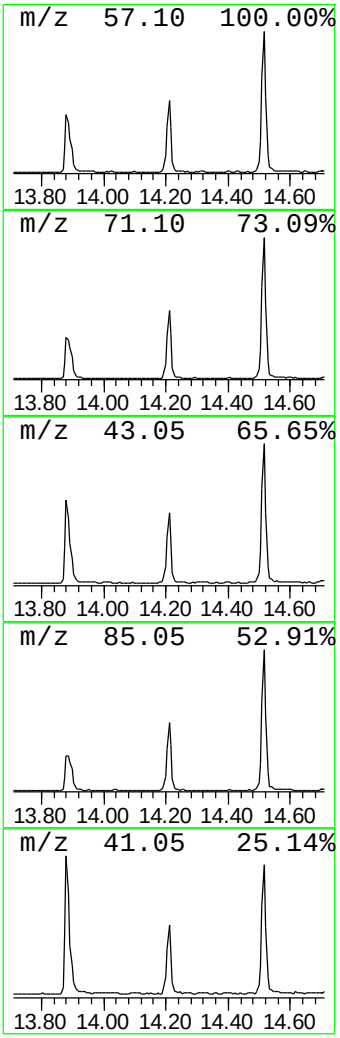
Peak Number 6 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	6.36 ng	1061290	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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Data File : BF118597.D
Acq On : 20 Jan 2020 18:04
Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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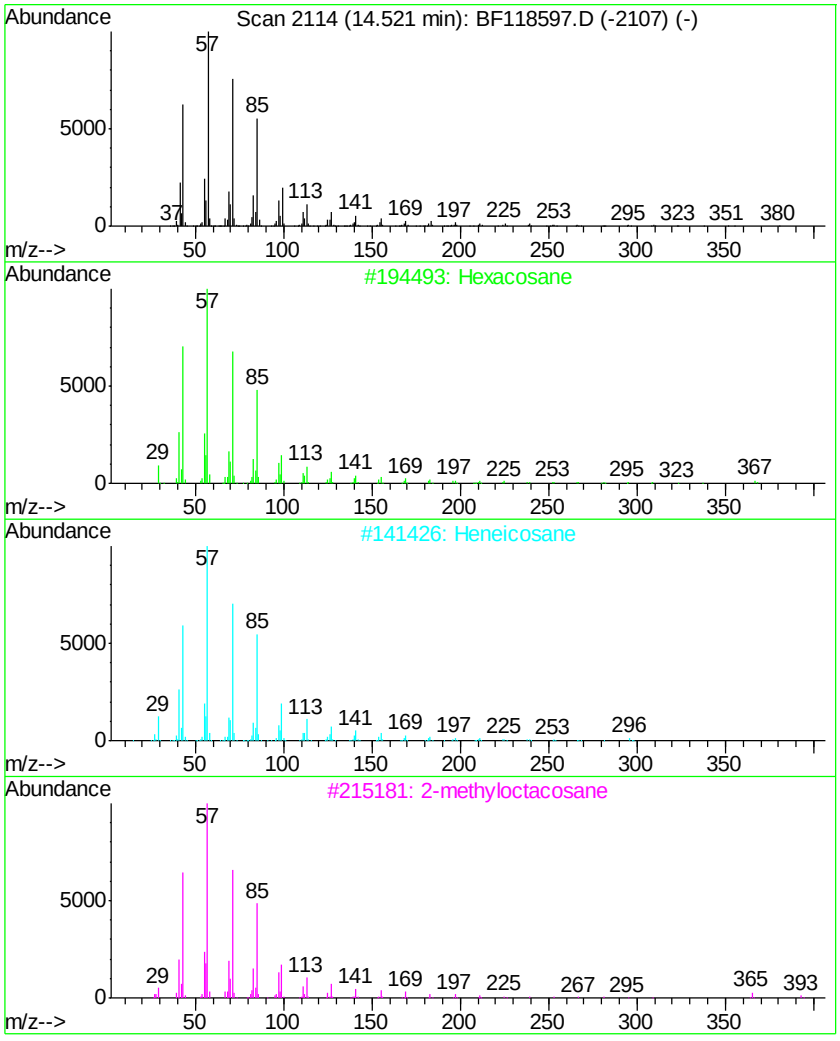
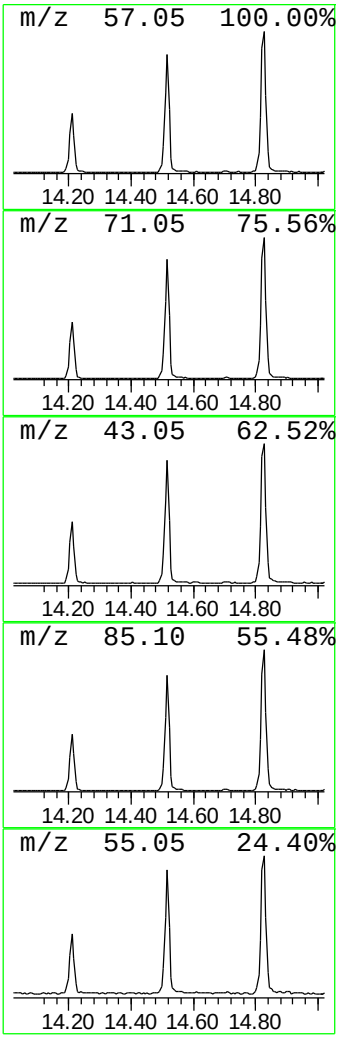
Peak Number 7 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	12.73 ng	2124450	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





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Instrument : BNA_F
ClientSampleId : PB126152BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

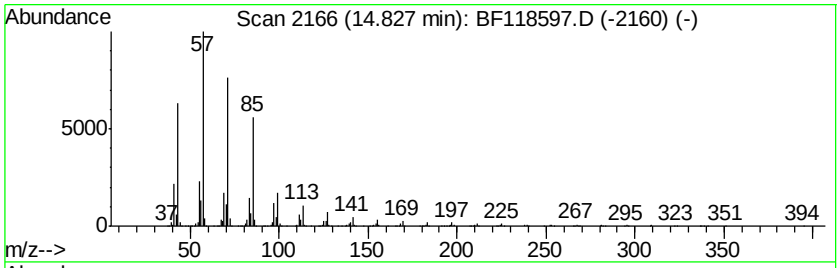
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

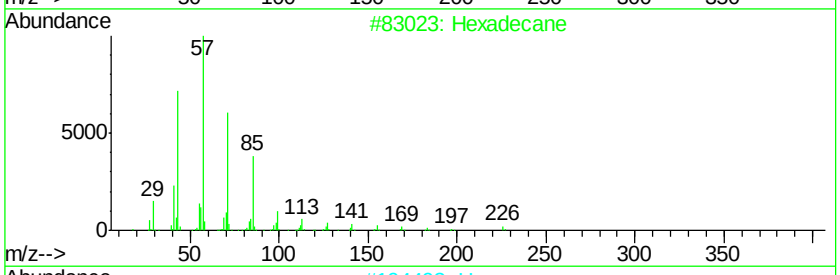
****

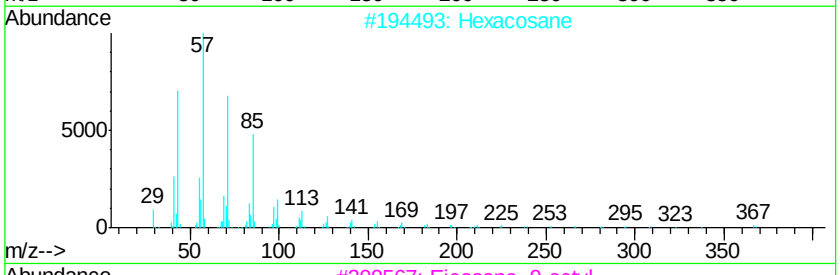
Peak Number 8 Hexadecane Concentration Rank 4

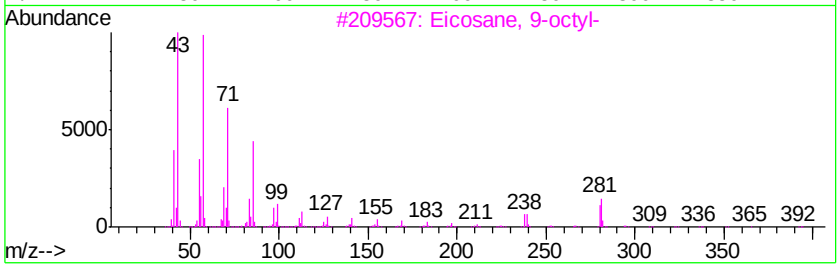
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	21.19 ng	2959110	Perylene-d12	15.51

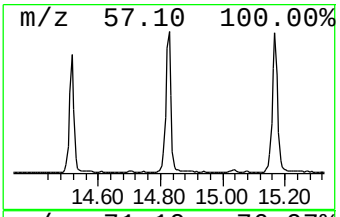
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Hexacosane	366	C26H54	000630-01-3	94
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	94
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
5	Heneicosane	296	C21H44	000629-94-7	91

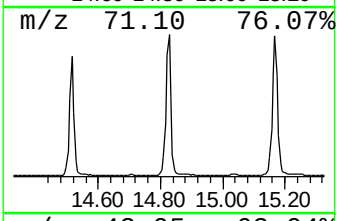


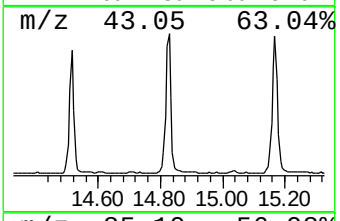


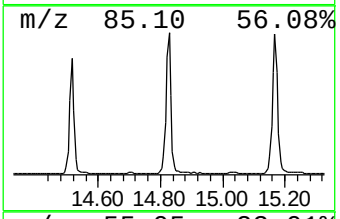


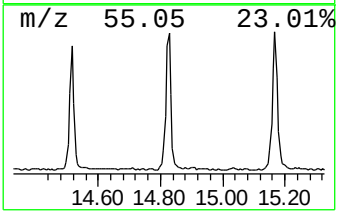












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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

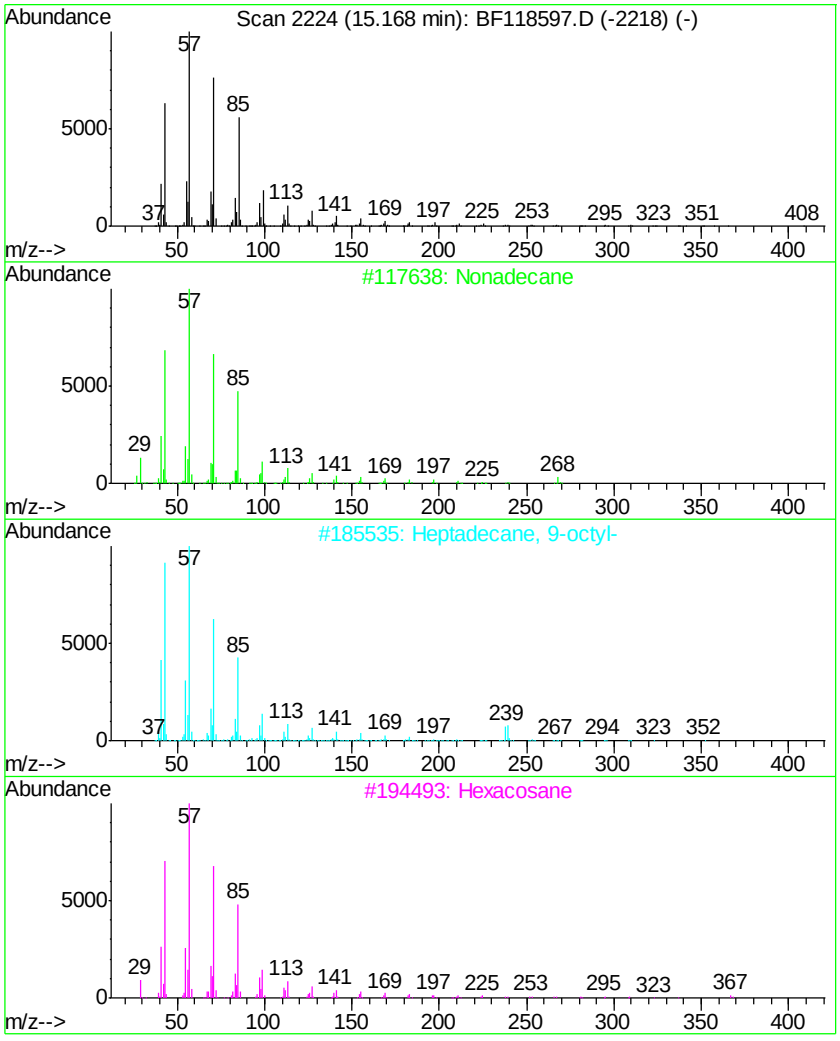
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

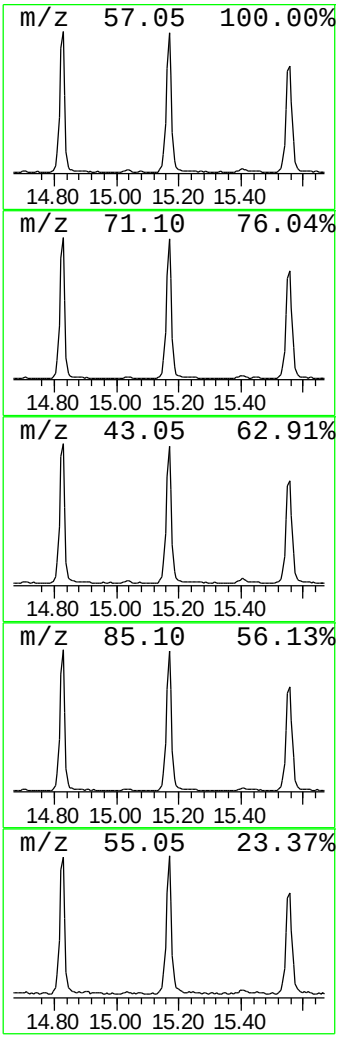
****

Peak Number 9 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	22.24 ng	3106750	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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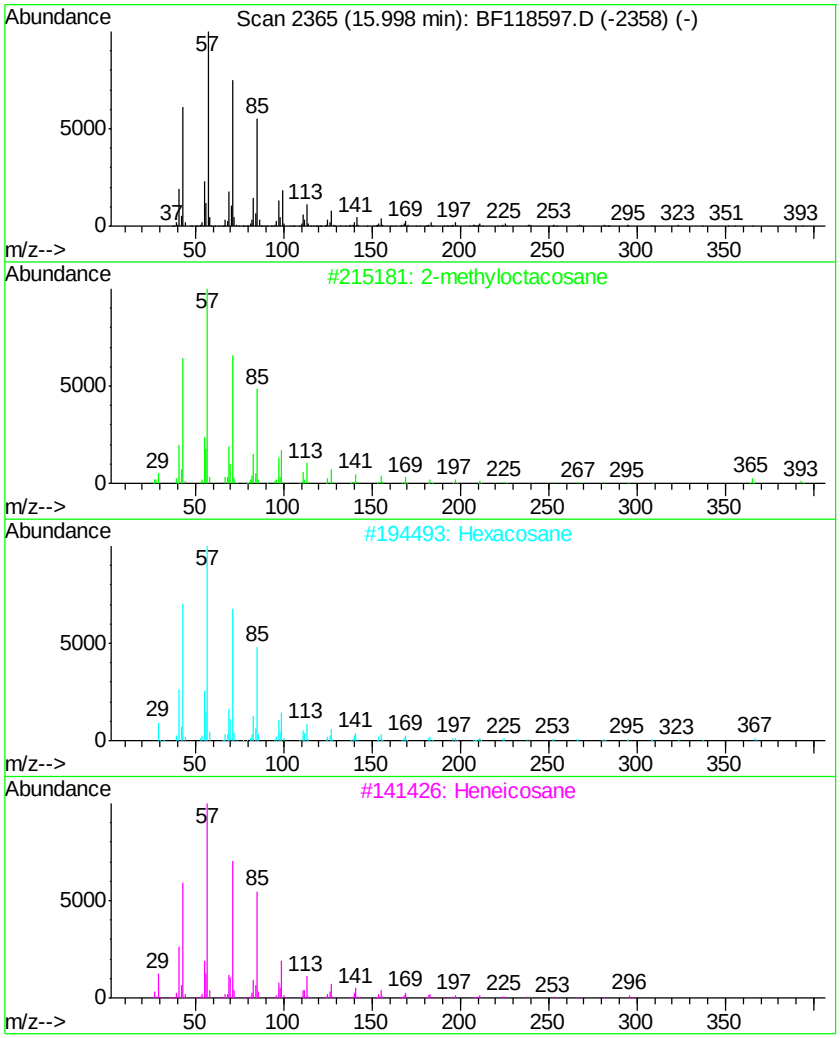
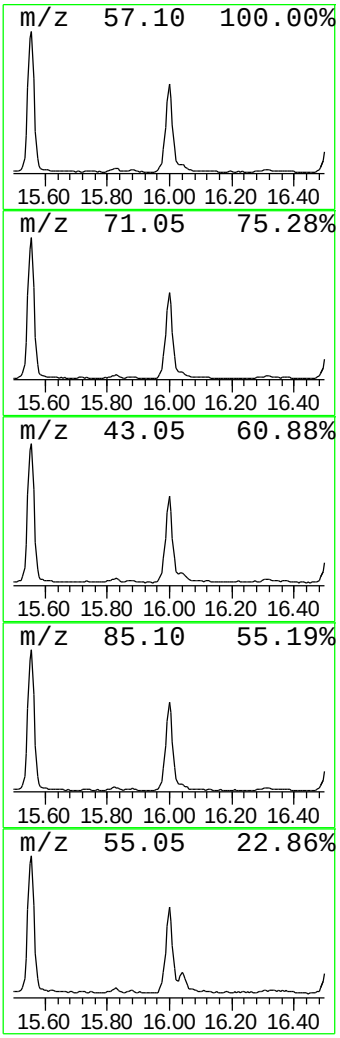
Peak Number 10 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	14.15 ng	1976000	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118597.D
Acq On : 20 Jan 2020 18:04
Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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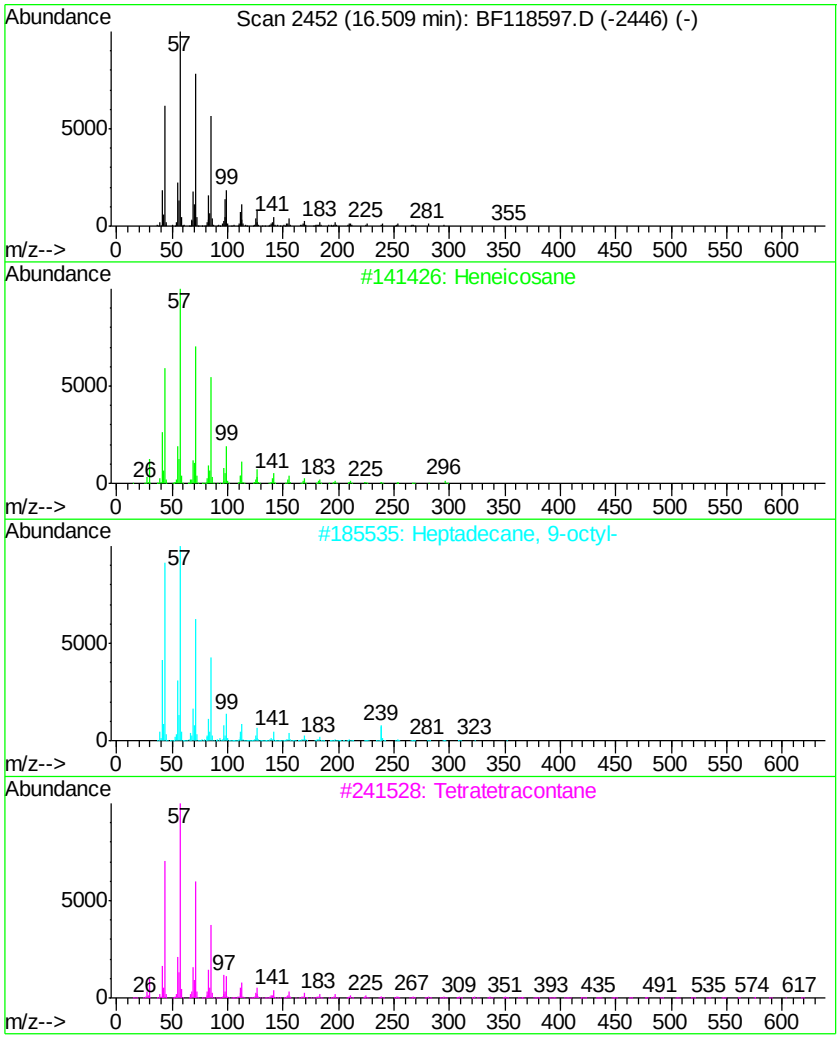
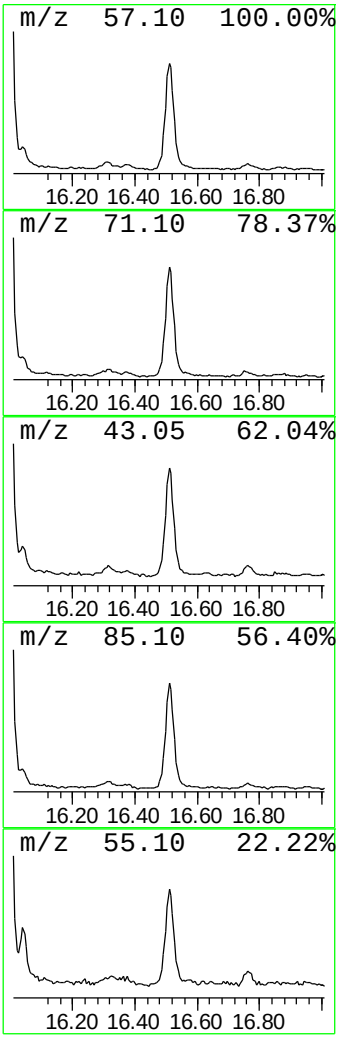
Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.51	7.27 ng	1016080	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012020\
Data File : BF118597.D
Acq On : 20 Jan 2020 18:04
Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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...	2.19	18.4	ng	2516040	1	6.88	2732960	20.0
2-Pentanone, 4-hy...	5.10	13.9	ng	1894040	1	6.88	2732960	20.0
unknown6.65	6.65	67.4	ng	9207870	1	6.88	2732960	20.0
1-Heneicosanol	13.88	12.5	ng	2087140	5	14.04	3337210	20.0
Heneicosane	14.21	6.4	ng	1061290	5	14.04	3337210	20.0
Hexacosane	14.52	12.7	ng	2124450	5	14.04	3337210	20.0
Hexadecane	14.83	21.2	ng	2959110	6	15.51	2793360	20.0
Nonadecane	15.17	22.2	ng	3106750	6	15.51	2793360	20.0
2-methyloctacosane	16.00	14.2	ng	1976000	6	15.51	2793360	20.0
Heptadecane, 9-oc...	16.51	7.3	ng	1016080	6	15.51	2793360	20.0