LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030920\
Data File : BF119284.D
Acq On : 9 Mar 2020 13:30
Operator : CG/JU
Sample : PB127331BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB127331BL

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-BF022020.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	2.669	95	99	107	rBV	141480	224811	3.37%	0.595%
2	4.516	410	413	423	rBV	61164	85922	1.29%	0.227%
3	4.957	484	488	503	rVB2	286573	498190	7.47%	1.318%
4	5.375	555	559	585	rBV	3050044	3450110	51.72%	9.130%
5	6.387	727	731	748	rBV	2770796	3140286	47.07%	8.310%
6	6.722	785	788	799	rVB	819436	787234	11.80%	2.083%
7	6.881	811	815	827	rBV	3523265	3310749	49.63%	8.761%
8	7.293	880	885	888	rBV	2414891	2543662	38.13%	6.731%
9	8.004	1002	1006	1015	rBV	1081964	1050134	15.74%	2.779%
10	9.081	1183	1189	1201	rBV	4973701	5625317	84.33%	14.885%
11	9.475	1253	1256	1261	rBV	88668	91799	1.38%	0.243%
12	9.757	1299	1304	1320	rBV	1461029	1370972	20.55%	3.628%
13	10.557	1435	1440	1456	rBV	3536045	4117303	61.72%	10.895%
14	11.245	1553	1557	1565	rBV	1523614	1470897	22.05%	3.892%
15	11.775	1644	1647	1659	rBV	338602	407052	6.10%	1.077%
16	12.557	1777	1780	1791	rBV3	45160	77840	1.17%	0.206%
17	12.645	1791	1795	1798	rVB2	82744	72149	1.08%	0.191%
18	12.833	1821	1827	1830	rBV	5890628	6670847	100.00%	17.652%
19	13.757	1980	1984	1997	rVB4	107590	252983	3.79%	0.669%
20	13.880	2002	2005	2016	rVB	1125456	1159127	17.38%	3.067%
21	14.633	2129	2133	2137	rVB2	87906	84746	1.27%	0.224%
22	14.704	2141	2145	2149	rBV	292001	272341	4.08%	0.721%
23	14.951	2183	2187	2192	rBV	74594	82186	1.23%	0.217%
24	15.310	2242	2248	2260	rBV	647239	943994	14.15%	2.498%

Sum of corrected areas: 37790651

LSC Report - Integrated Chromatogram

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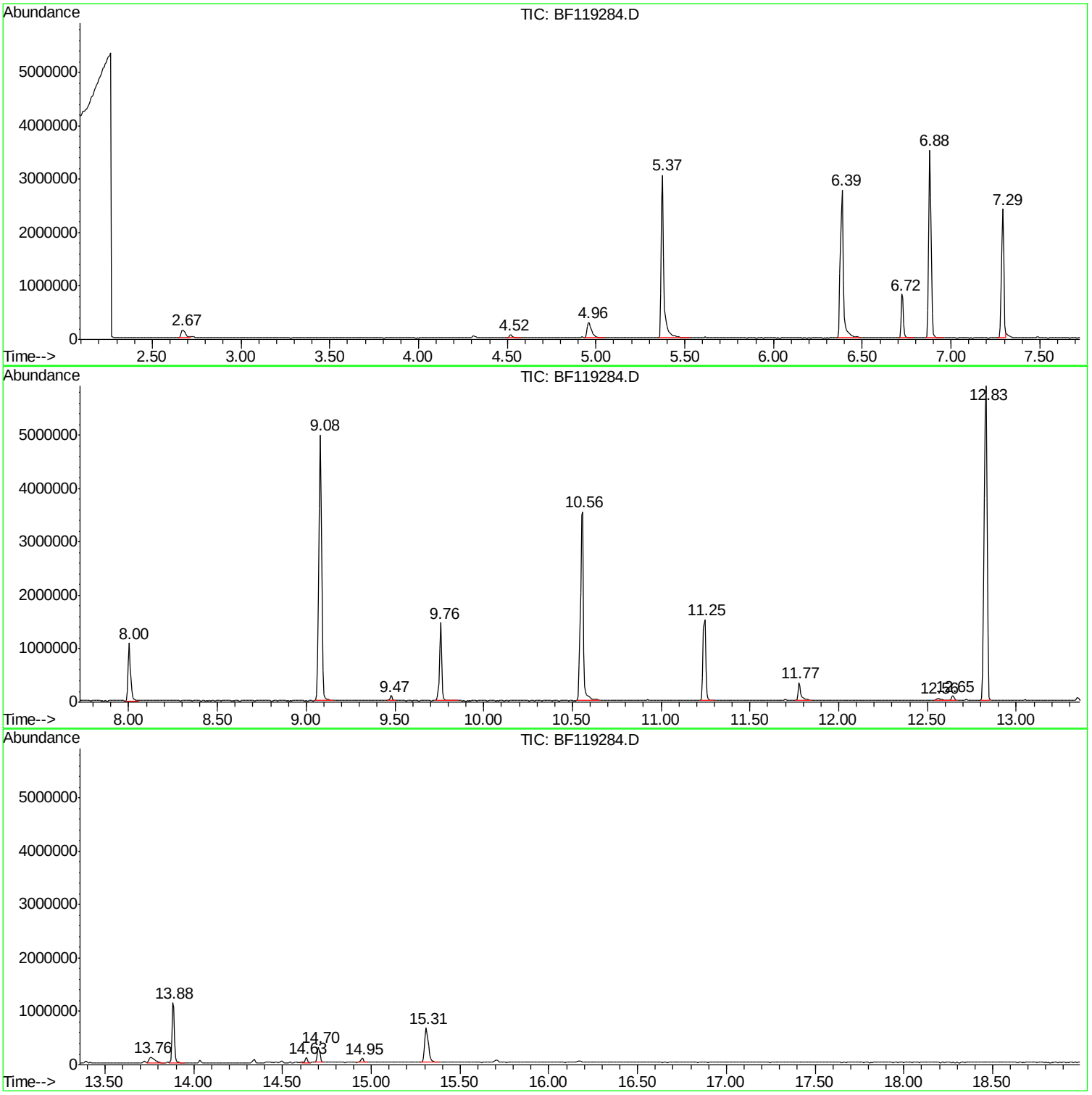
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB127331BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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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Sample : PB127331BL
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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB127331BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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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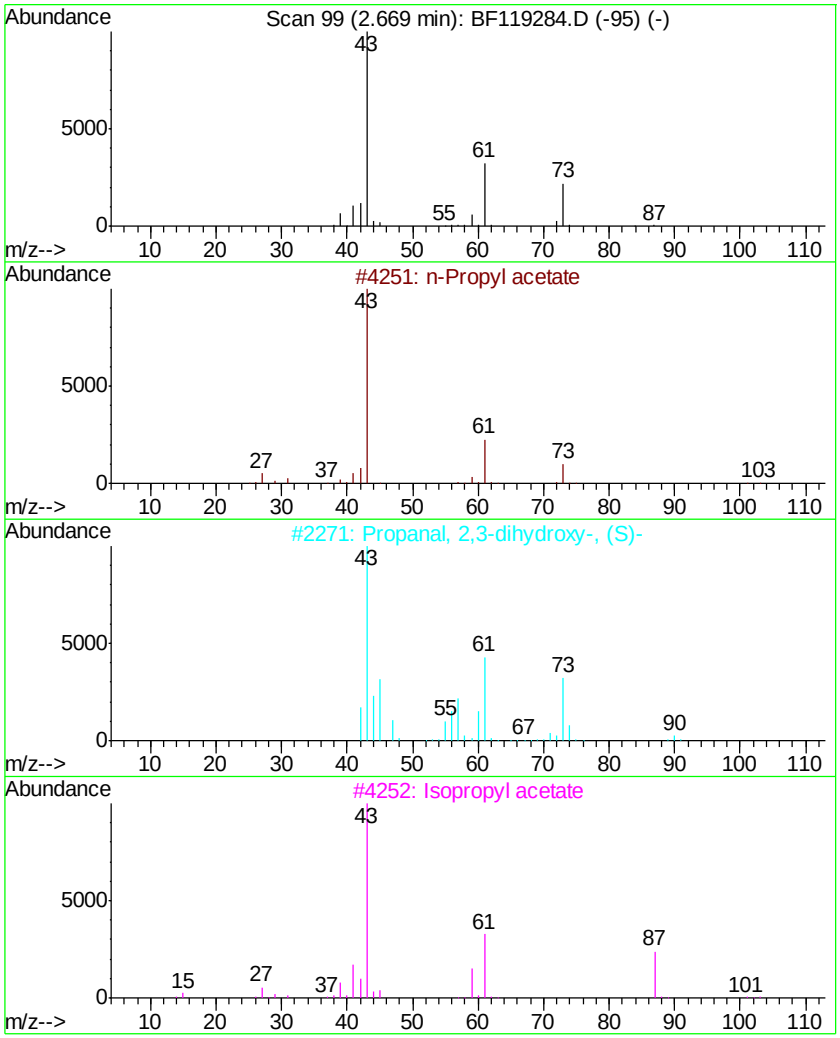
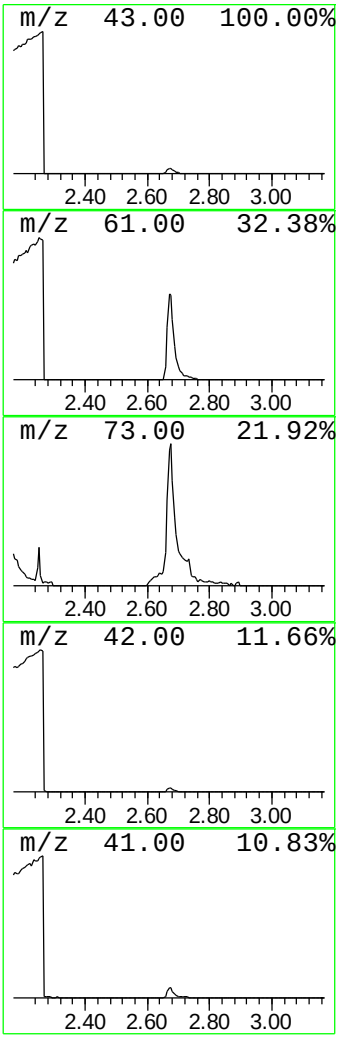
Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.67	5.71 ng	224811	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	64
2	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38
3	Isopropyl acetate	102	C5H10O2	000108-21-4	28
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9





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Data File : BF119284.D
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Operator : CG/JU
Sample : PB127331BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB127331BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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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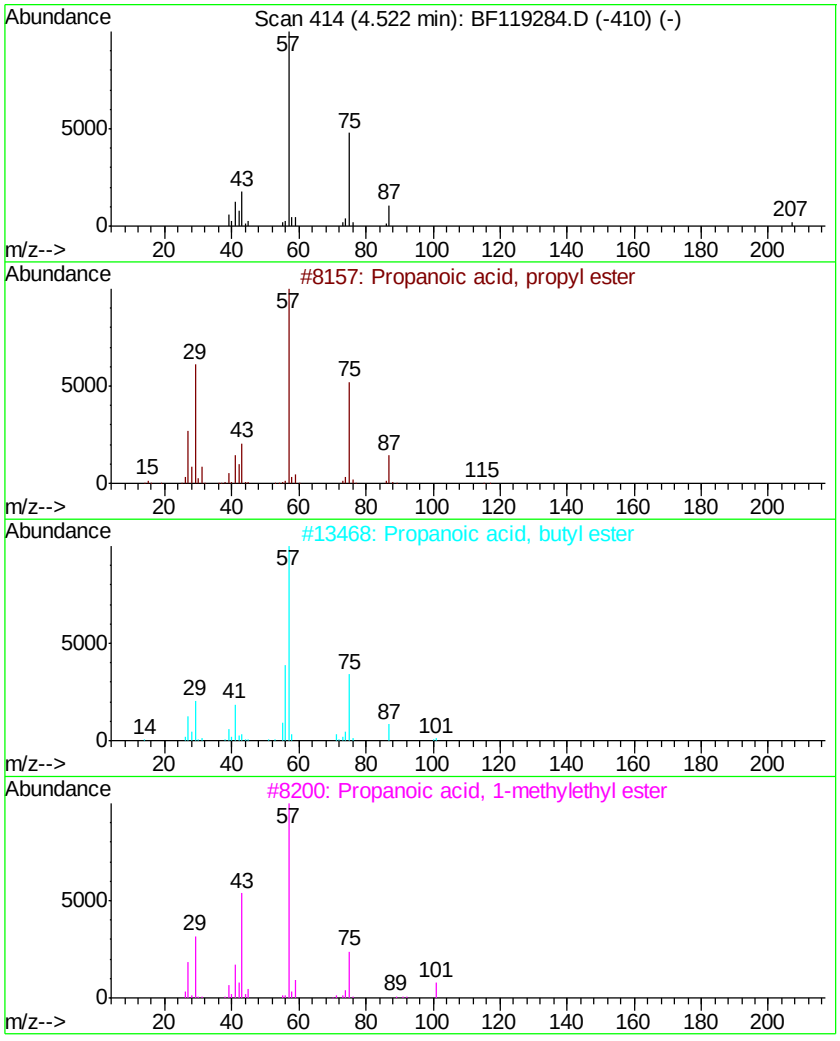
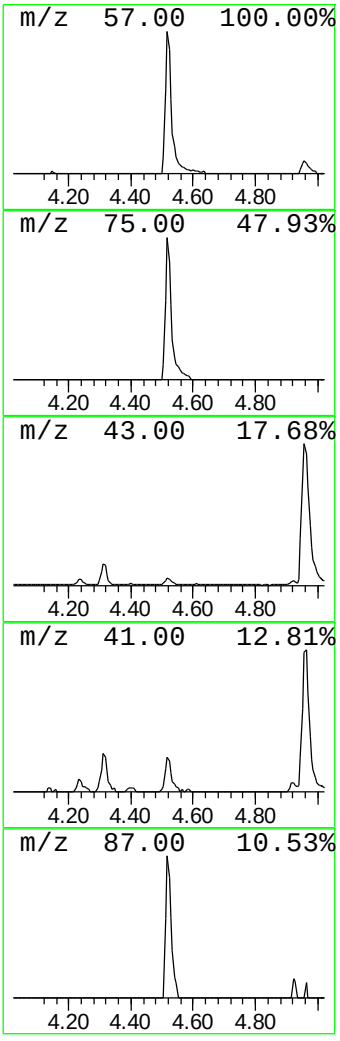
Peak Number 2 Propanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	2.18 ng	85922	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	23
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





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Data File : BF119284.D
Acq On : 9 Mar 2020 13:30
Operator : CG/JU
Sample : PB127331BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB127331BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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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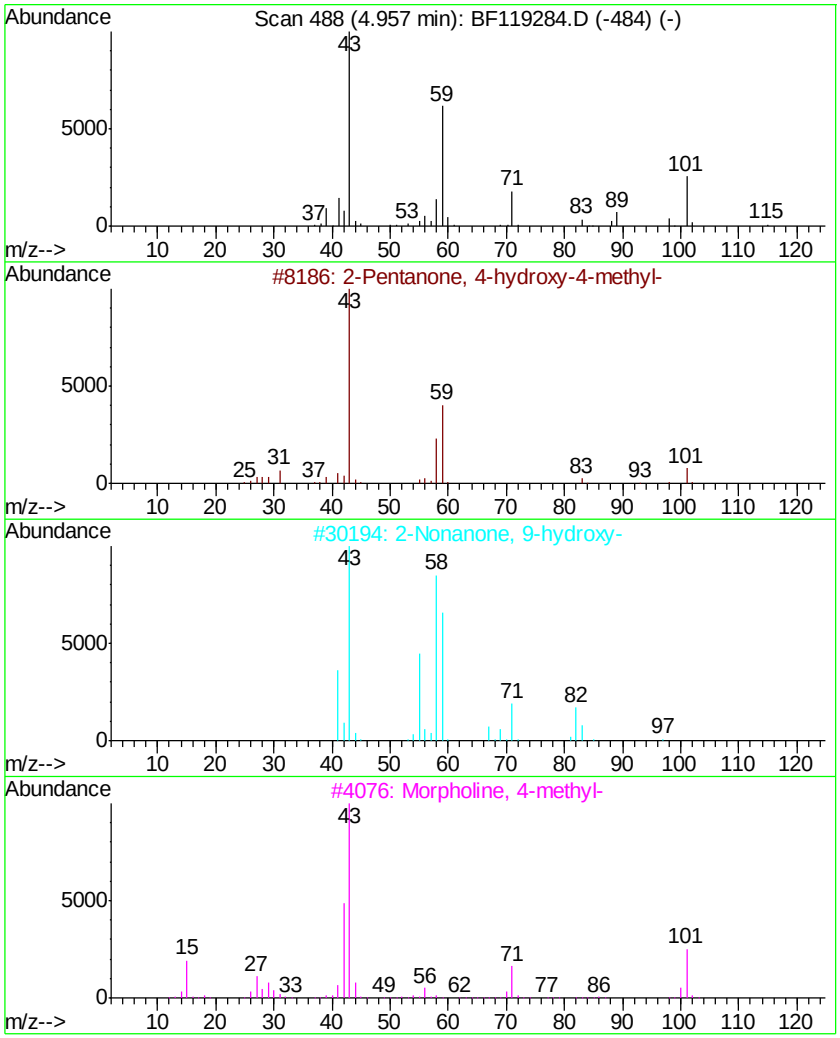
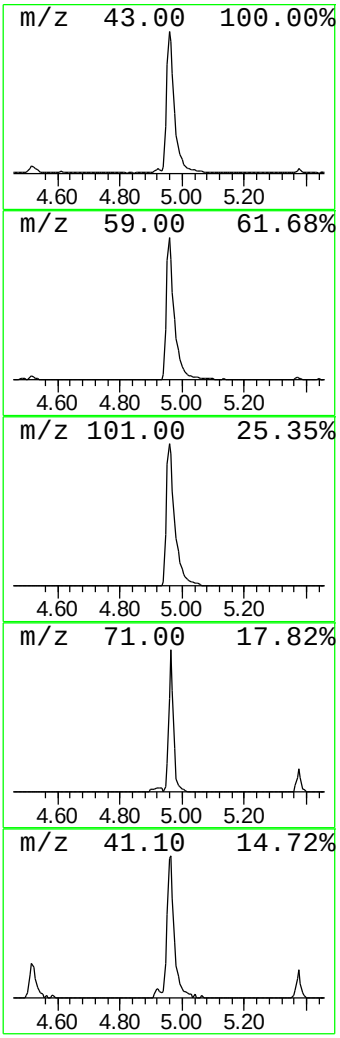
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	12.66 ng	498190	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	25
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	25
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	23





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030920\
Data File : BF119284.D
Acq On : 9 Mar 2020 13:30
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Sample : PB127331BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB127331BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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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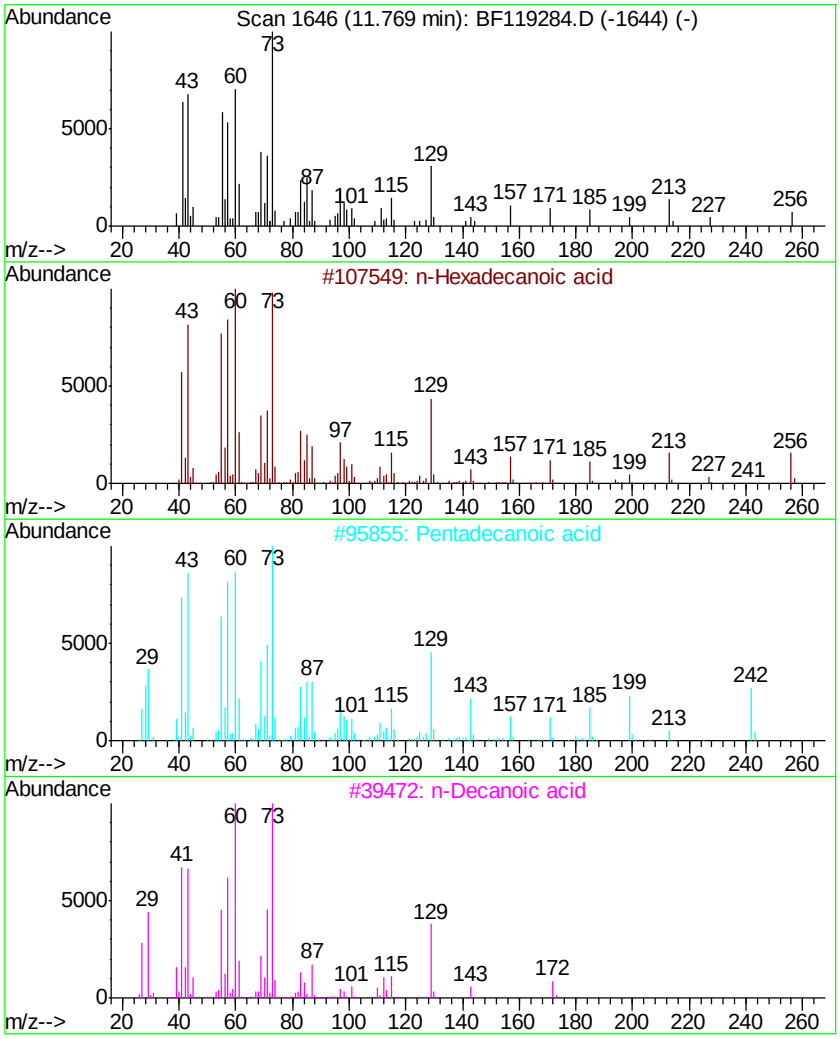
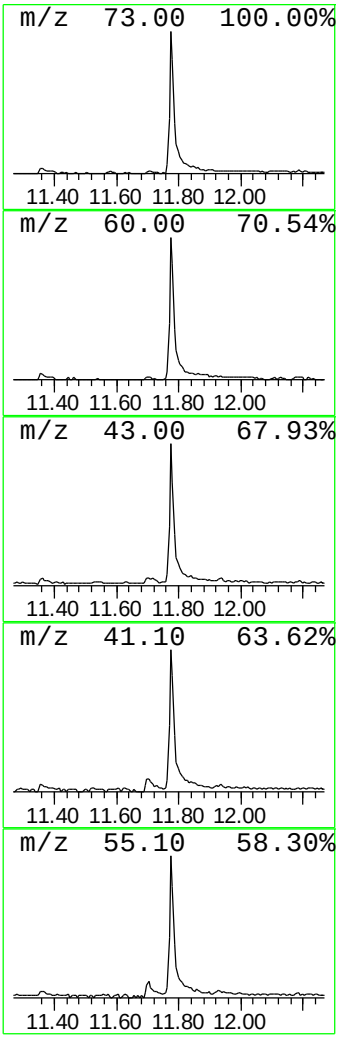
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	5.53 ng	407052	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	25





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Instrument : BNA_F
ClientSampleId : PB127331BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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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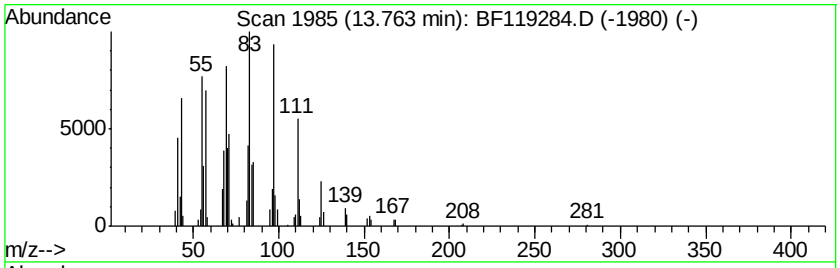
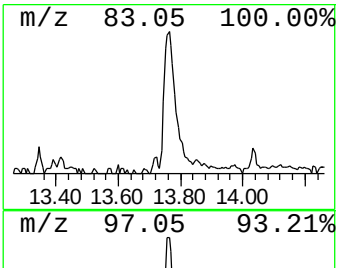
Peak Number 6 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	4.37 ng	252983	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91





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ClientSampleId : PB127331BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

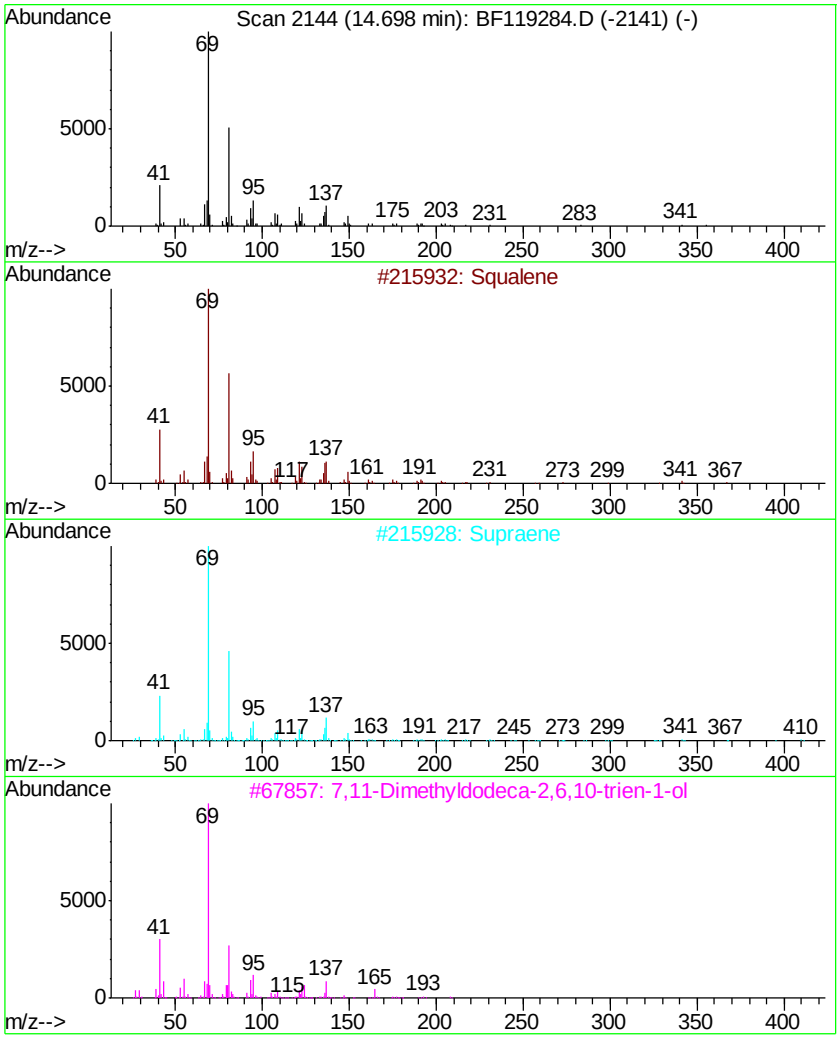
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

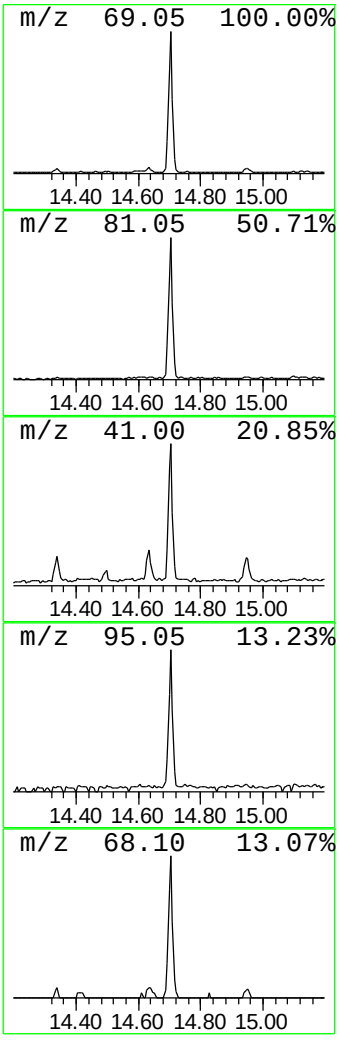
****

Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	5.77 ng	272341	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50
5	Methacrylic acid, 2,3-dimethylph...	190	C12H14O2	1000360-69-2	47





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.67	5.7	ng	224811	1	6.72	787234	20.0
Propanoic acid, p...	4.52	2.2	ng	85922	1	6.72	787234	20.0
2-Pentanone, 4-hy...	4.96	12.7	ng	498190	1	6.72	787234	20.0
n-Hexadecanoic acid	11.77	5.5	ng	407052	4	11.25	1470900	20.0
n-Nonadecanol-1	13.76	4.4	ng	252983	5	13.88	1159130	20.0
Squalene	14.70	5.8	ng	272341	6	15.31	943994	20.0