LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005931.D
Acq On : 15 Jun 2021 15:29
Operator : CG/JU
Sample : M2672-16
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(68-72)

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_P\Methods\8270E-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	16	rVB	104465	116816	2.69%	0.571%
2	5.505	404	411	417	rBV	1117078	1627237	37.48%	7.950%
3	5.564	417	421	433	rVB	41610	88077	2.03%	0.430%
4	7.105	676	683	695	rBV	993089	1624191	37.41%	7.935%
5	7.934	816	824	832	rBV	259012	417198	9.61%	2.038%
6	9.099	1014	1022	1037	rVB	623254	1024159	23.59%	5.004%
7	10.534	1259	1266	1273	rBV2	19606	45249	1.04%	0.221%
8	10.740	1291	1301	1313	rBV	307655	534341	12.31%	2.611%
9	13.187	1710	1717	1731	rBV	1652186	2508033	57.77%	12.253%
10	14.422	1917	1927	1932	rBV4	26674	73014	1.68%	0.357%
11	14.563	1944	1951	1963	rVB	487774	729667	16.81%	3.565%
12	15.381	2085	2090	2103	rVB	25751	52929	1.22%	0.259%
13	15.969	2185	2190	2195	rBV	61801	80234	1.85%	0.392%
14	16.045	2197	2203	2225	rVV	1612423	2435267	56.09%	11.898%
15	17.304	2411	2417	2425	rBV	603509	882312	20.32%	4.311%
16	17.428	2432	2438	2443	rVB4	50303	72261	1.66%	0.353%
17	18.186	2563	2567	2574	rBV2	69229	108106	2.49%	0.528%
18	19.416	2772	2776	2782	rBV3	39023	54058	1.25%	0.264%
19	19.857	2845	2851	2857	rBV	3539378	4341479	100.00%	21.211%
20	20.522	2958	2964	2970	rBV	289496	360859	8.31%	1.763%
21	20.592	2972	2976	2979	rBV	91876	102588	2.36%	0.501%
22	21.080	3056	3059	3068	rBV2	115271	180317	4.15%	0.881%
23	21.280	3090	3093	3098	rVB	108413	126622	2.92%	0.619%
24	21.380	3105	3110	3117	rBV	961090	1251813	28.83%	6.116%
25	22.480	3293	3297	3303	rVB	121123	174087	4.01%	0.851%
26	23.792	3514	3520	3530	rVB2	693812	1457063	33.56%	7.119%

Sum of corrected areas: 20467977

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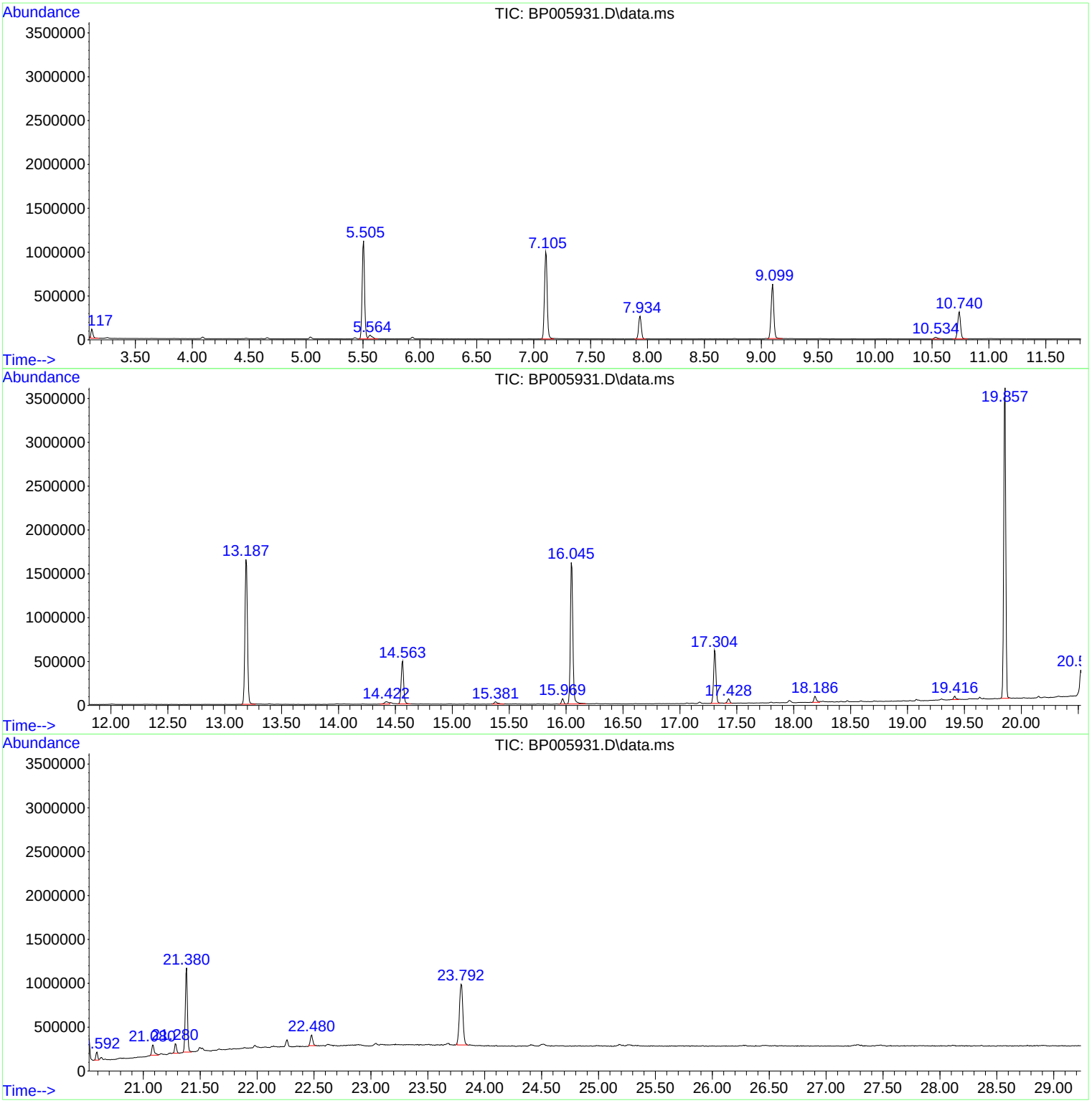
ClientSampleId :
17-B6(68-72)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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TIC Integration Parameters: LSCINT.P

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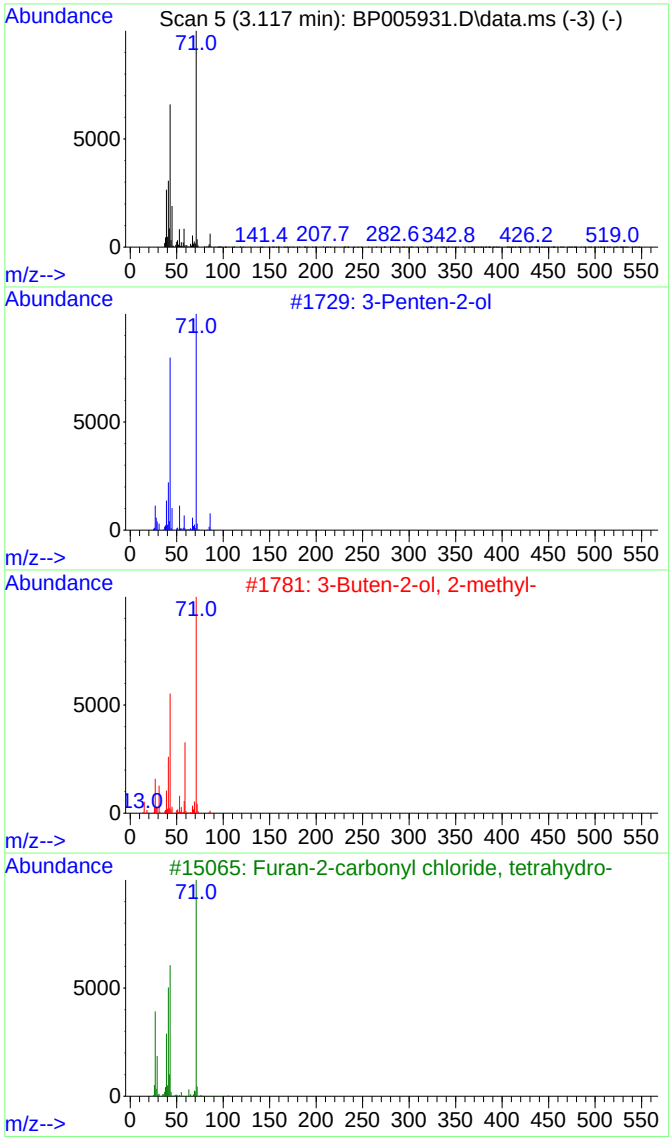
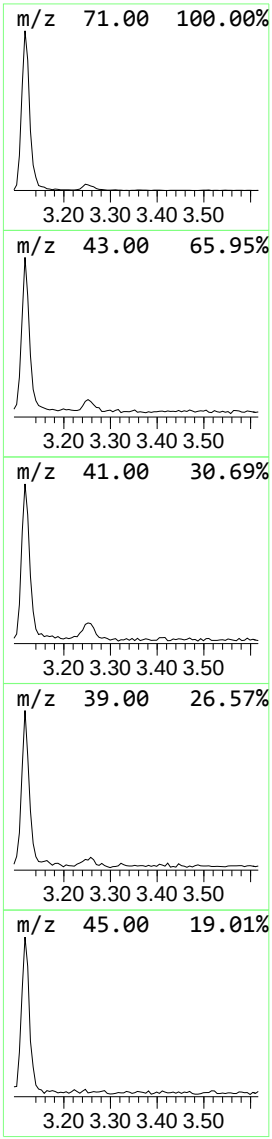
Peak Number 1 3-Penten-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	5.60 ng	116816	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	83
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	59
3	Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	59
4	Acetic acid, (1,2-dimethyl-1-pro...	128	C7H12O2	003814-41-3	45
5	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	45





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Instrument :
BNA_P
ClientSampleId :
17-B6(68-72)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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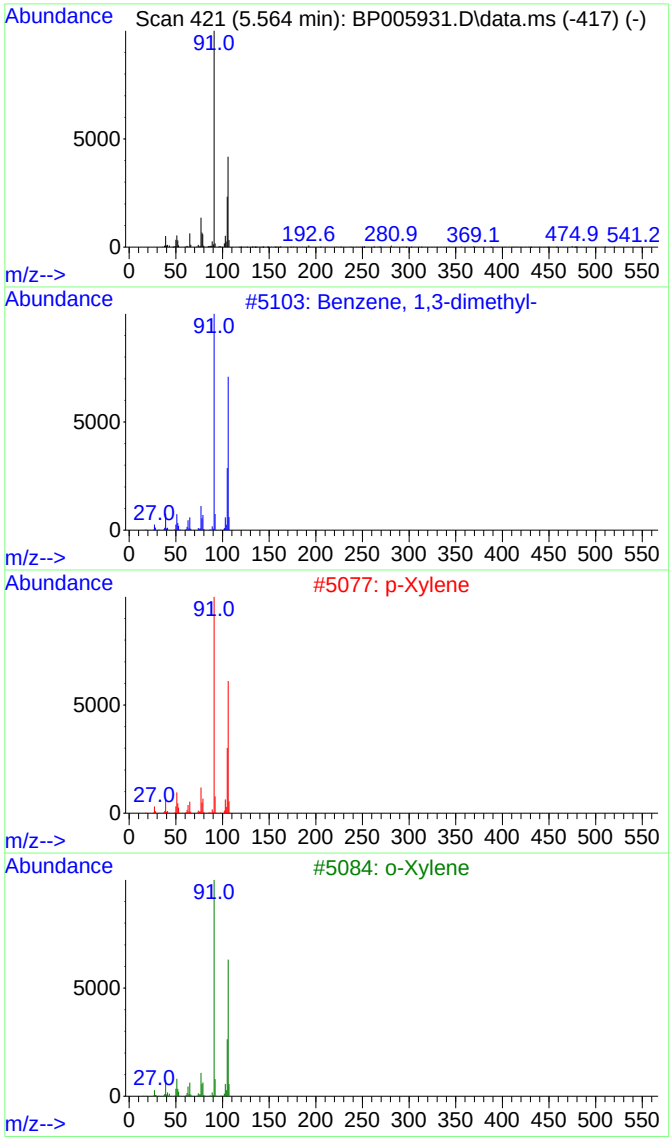
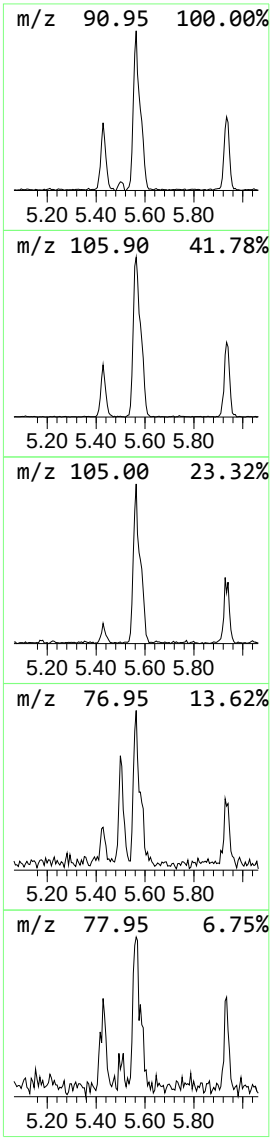
Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.564	4.22 ng	88077	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	90
2	p-Xylene	106	C8H10	000106-42-3	90
3	o-Xylene	106	C8H10	000095-47-6	90
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	78
5	Benzeneethanol, .alpha.,.beta.-d...	150	C10H14O	052089-32-4	64





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Data File : BP005931.D
Acq On : 15 Jun 2021 15:29
Operator : CG/JU
Sample : M2672-16
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(68-72)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
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TIC Integration Parameters: LSCINT.P

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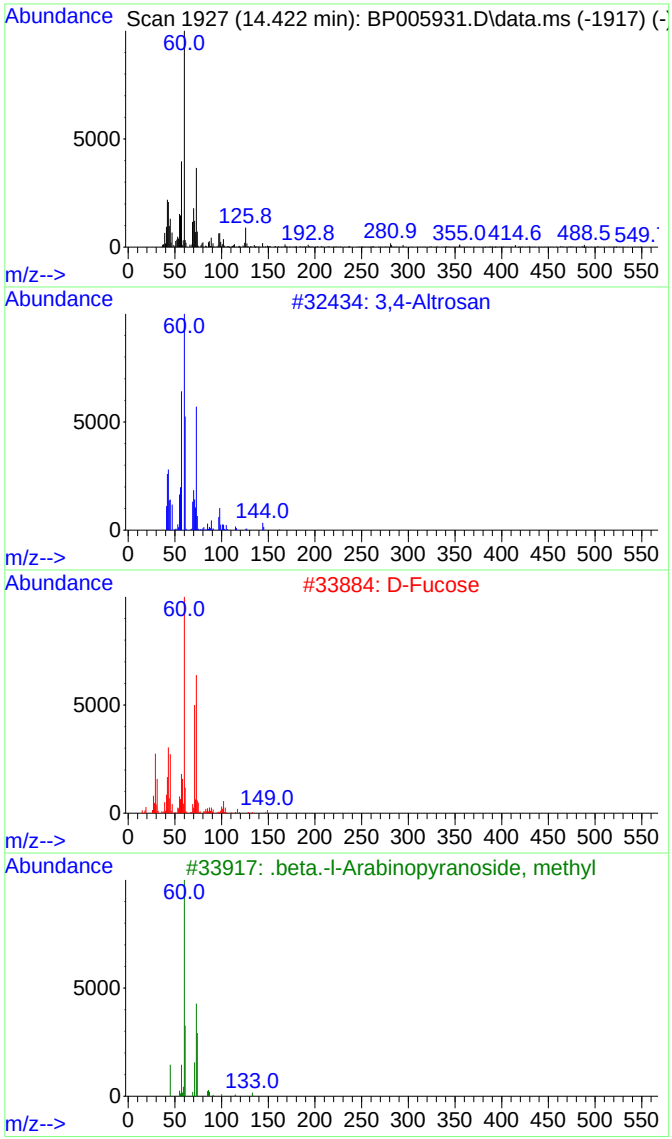
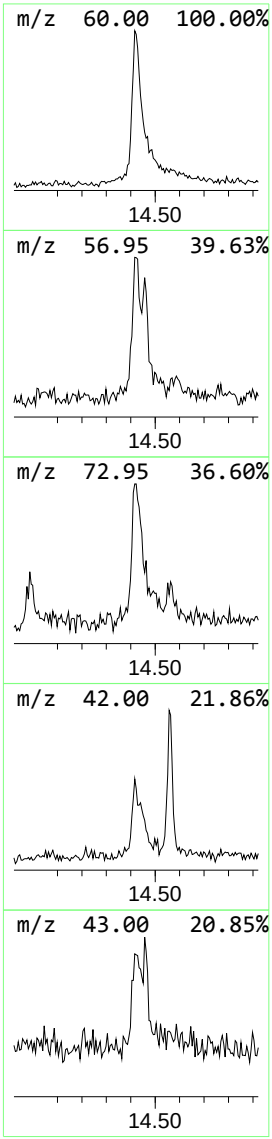
Peak Number 3 3,4-Altrosan Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	2.00 ng	73014	Acenaphthene-d10	14.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Altrosan	162	C6H10O5	1000129-76-4	90
2	D-Fucose	164	C6H12O5	003615-37-0	64
3	.beta.-l-Arabinopyranoside, methyl	164	C6H12O5	001825-00-9	64
4	Hexanoic acid	116	C6H12O2	000142-62-1	59
5	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	56





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BNA_P
ClientSampleId :
17-B6(68-72)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
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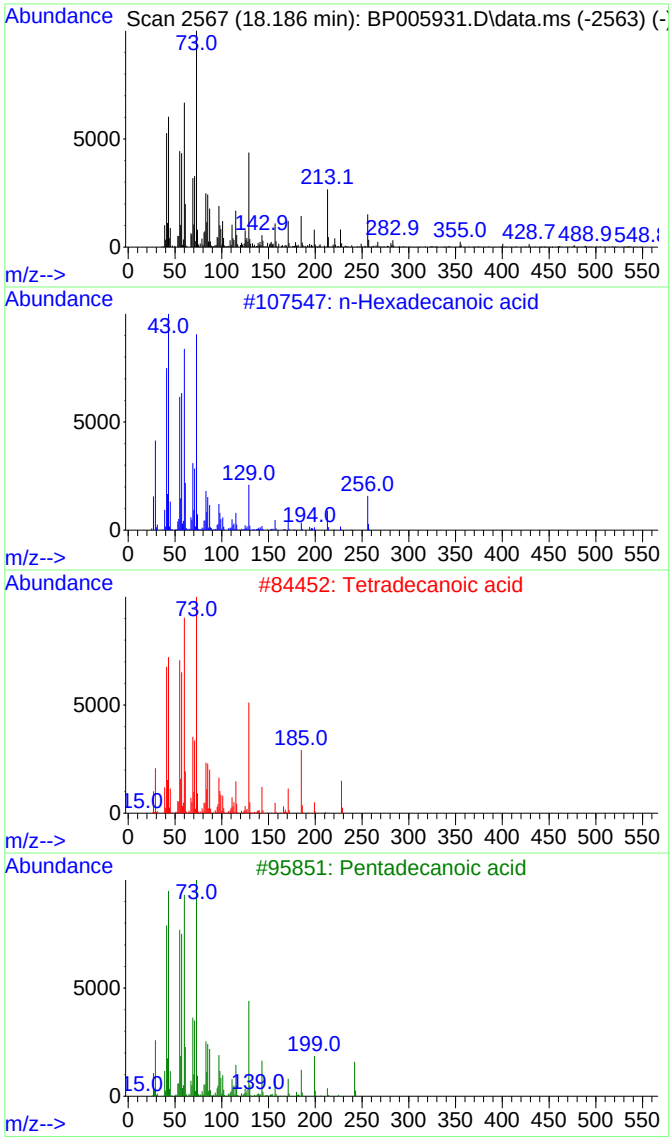
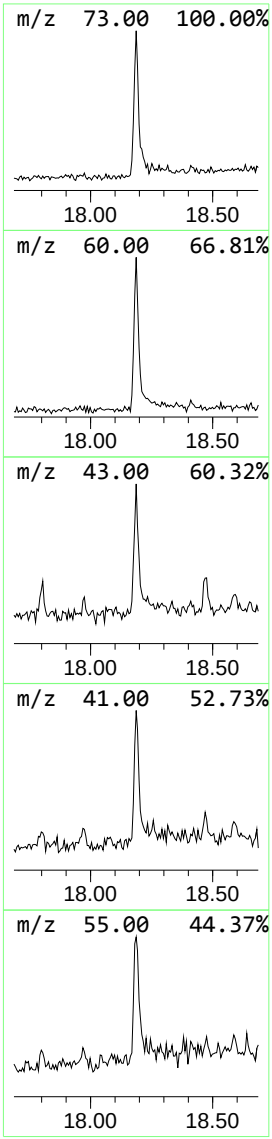
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	2.45 ng	108106	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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17-B6(68-72)

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

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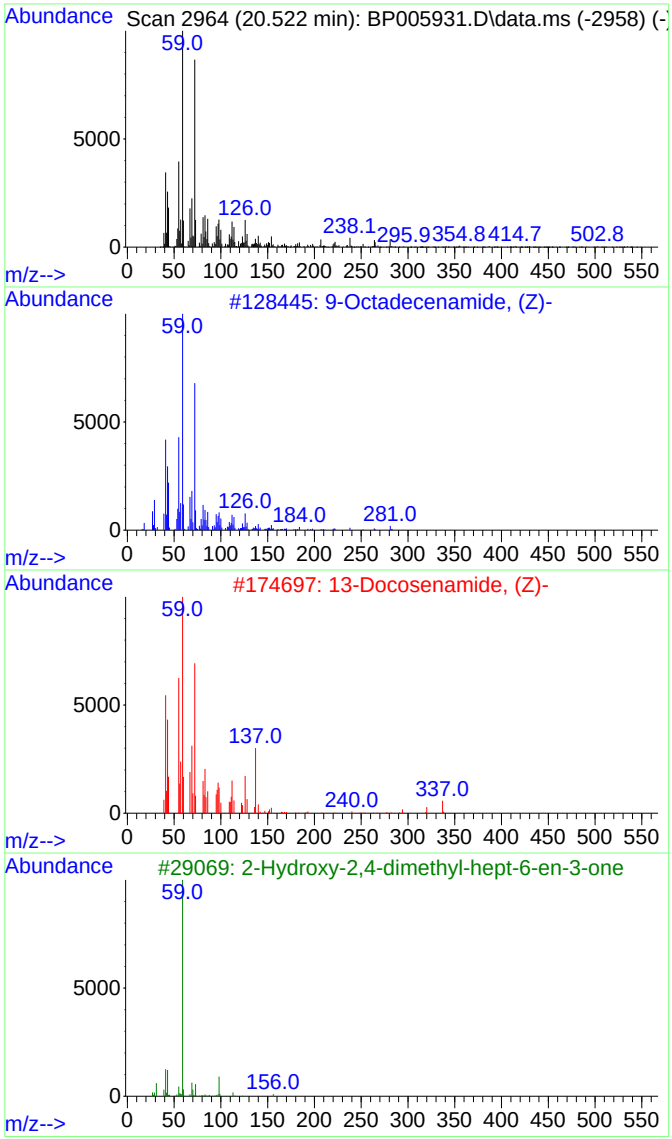
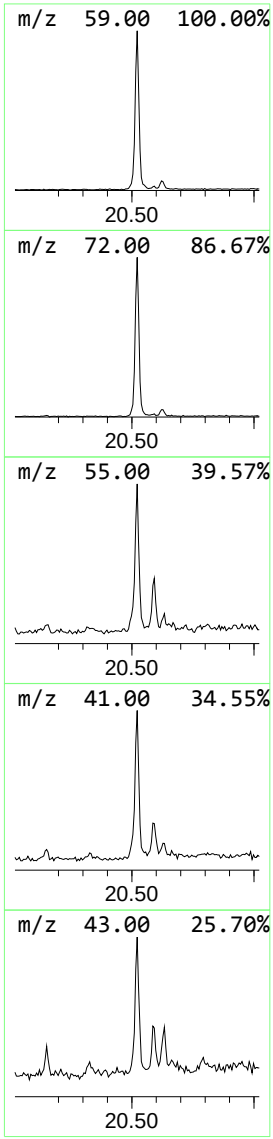
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.522	5.77 ng	360859	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	43
3	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	30
4	Urea, 1-butyl-3-(propylsulfonyl)...	238	C8H18N2O2S2	024539-91-1	27
5	Bicyclo[3.2.1]heptane, 1-methoxy-	126	C8H14O	1000156-43-7	27





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Instrument :
BNA_P
ClientSampleId :
17-B6(68-72)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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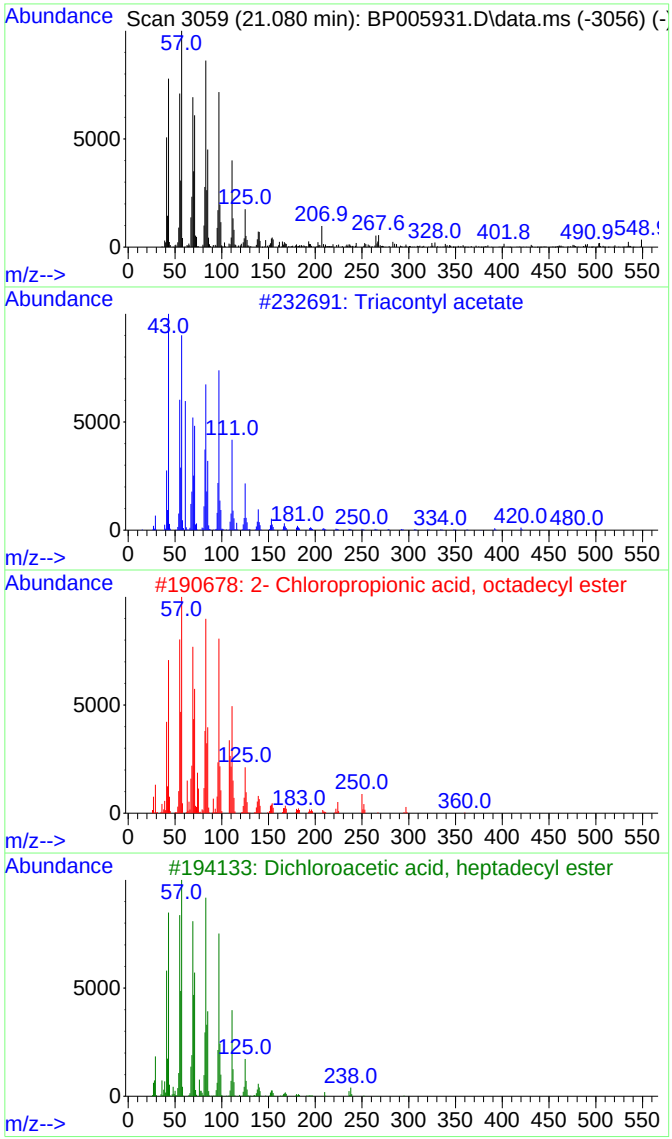
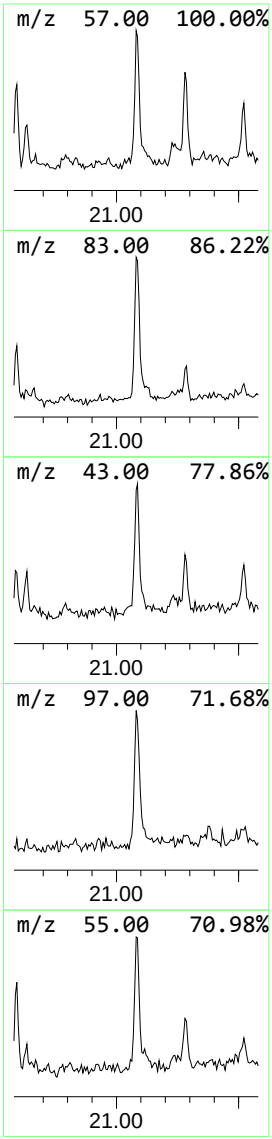
Peak Number 6 Triacontyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	2.88 ng	180317	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontyl acetate	480	C32H64O2	041755-58-2	96
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

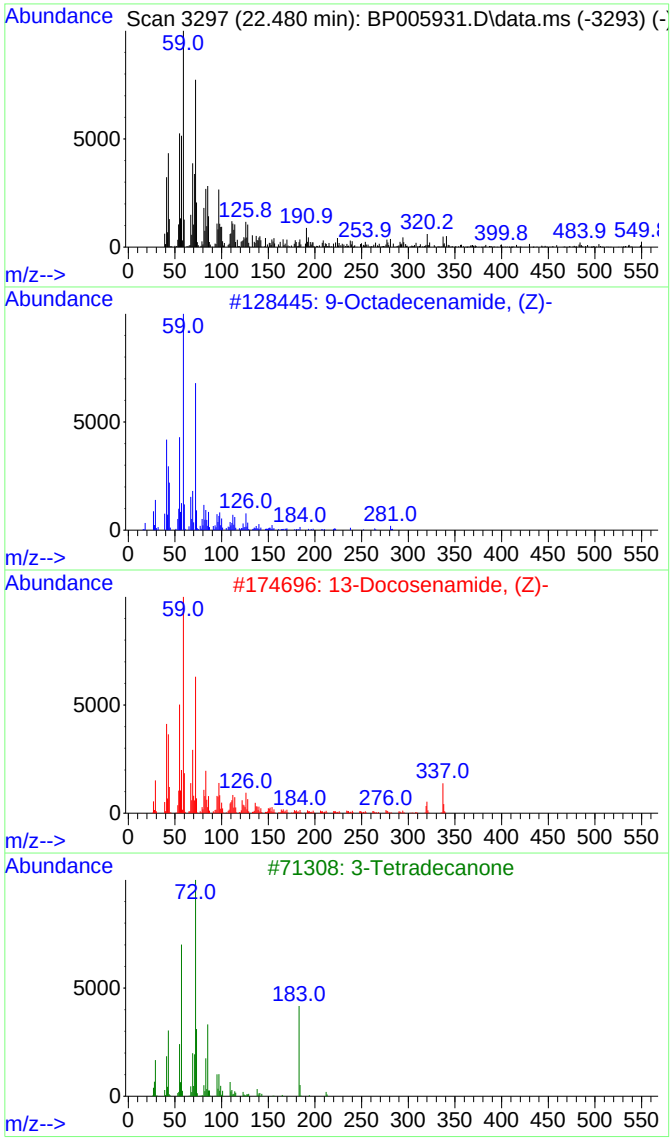
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

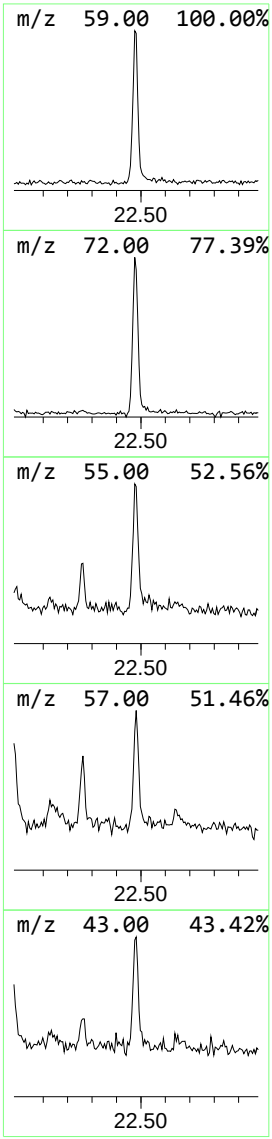
****

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.480	2.78 ng	174087	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	55
3	3-Tetradecanone	212	C14H28O	000629-23-2	45
4	3-Dodecanone	184	C12H24O	001534-27-6	43
5	Dodecanamide	199	C12H25NO	001120-16-7	43





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-ol	3.117	5.6	ng	116816	1	7.934	417198	20.0
Benzene, 1,3-di...	5.564	4.2	ng	88077	1	7.934	417198	20.0
3,4-Altrosan	14.422	2.0	ng	73014	3	14.563	729667	20.0
n-Hexadecanoic ...	18.186	2.5	ng	108106	4	17.304	882312	20.0
9-Octadecenamid...	20.522	5.8	ng	360859	5	21.380	1251810	20.0
Triacontyl acetate	21.080	2.9	ng	180317	5	21.380	1251810	20.0
13-Docosenamide...	22.480	2.8	ng	174087	5	21.380	1251810	20.0