LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

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\8270-BP091520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003337.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.340	73	77	92	rVB	98584	138215	1.81%	0.252%
2	5.187	379	391	409	rBV	2092087	3166349	41.38%	5.780%
3	6.769	653	660	685	rBV	2022324	3314373	43.32%	6.050%
4	7.181	724	730	743	rBV	59790	105078	1.37%	0.192%
5	7.569	789	796	806	rBV	641950	981653	12.83%	1.792%
6	8.722	984	992	1005	rBV	1372196	2273552	29.71%	4.150%
7	10.346	1261	1268	1284	rBV	880468	1489503	19.47%	2.719%
8	12.840	1684	1692	1711	rBV	3366120	5086909	66.48%	9.285%
9	13.140	1738	1743	1761	rBV2	26830	77722	1.02%	0.142%
10	13.681	1829	1835	1847	rBV	492118	687020	8.98%	1.254%
11	14.222	1920	1927	1939	rBV	1428808	2126670	27.80%	3.882%
12	15.716	2173	2181	2203	rBV	2749194	4182265	54.66%	7.634%
13	16.975	2389	2395	2408	rVB	1800991	2523082	32.98%	4.605%
14	17.898	2547	2552	2559	rBV	197915	320924	4.19%	0.586%
15	18.939	2726	2729	2735	rBV	64705	81164	1.06%	0.148%
16	19.139	2759	2763	2767	rBV	72402	114475	1.50%	0.209%
17	19.557	2828	2834	2845	rVB	5821273	7651258	100.00%	13.966%
18	20.351	2964	2969	2973	rBV3	64744	110548	1.44%	0.202%
19	20.739	3026	3035	3041	rBV3	204183	585840	7.66%	1.069%
20	20.798	3041	3045	3052	rVV2	942173	1295992	16.94%	2.366%
21	21.069	3086	3091	3103	rVB	2333728	2899123	37.89%	5.292%
22	21.233	3115	3119	3128	rVB	462044	485992	6.35%	0.887%
23	21.657	3186	3191	3197	rBV	975012	1212931	15.85%	2.214%
24	22.110	3263	3268	3281	rVB	1701344	2294722	29.99%	4.189%
25	22.233	3286	3289	3294	rVB	86881	111290	1.45%	0.203%
26	22.610	3347	3353	3369	rVB	1869045	3043470	39.78%	5.555%
27	23.168	3442	3448	3456	rBV	1590519	2775525	36.28%	5.066%
28	23.263	3457	3464	3475	rVB2	1432282	2698604	35.27%	4.926%
29	23.810	3550	3557	3565	rBV	944921	1915377	25.03%	3.496%
30	24.551	3676	3683	3702	rVB2	410765	1035407	13.53%	1.890%

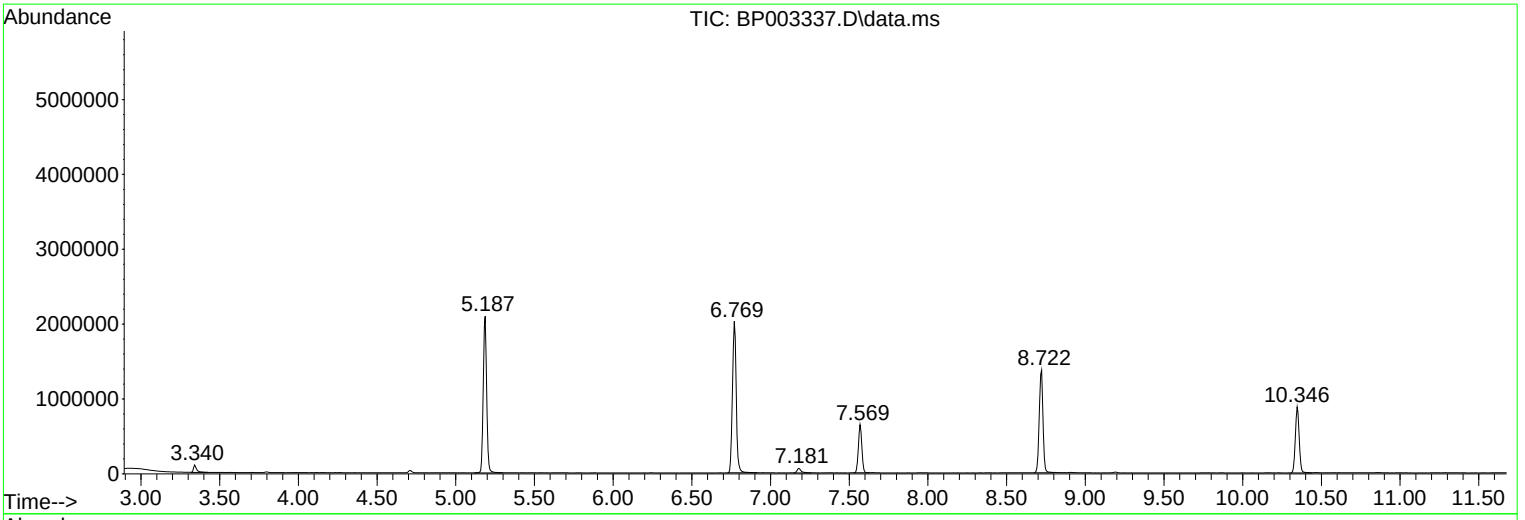
Sum of corrected areas: 54785033

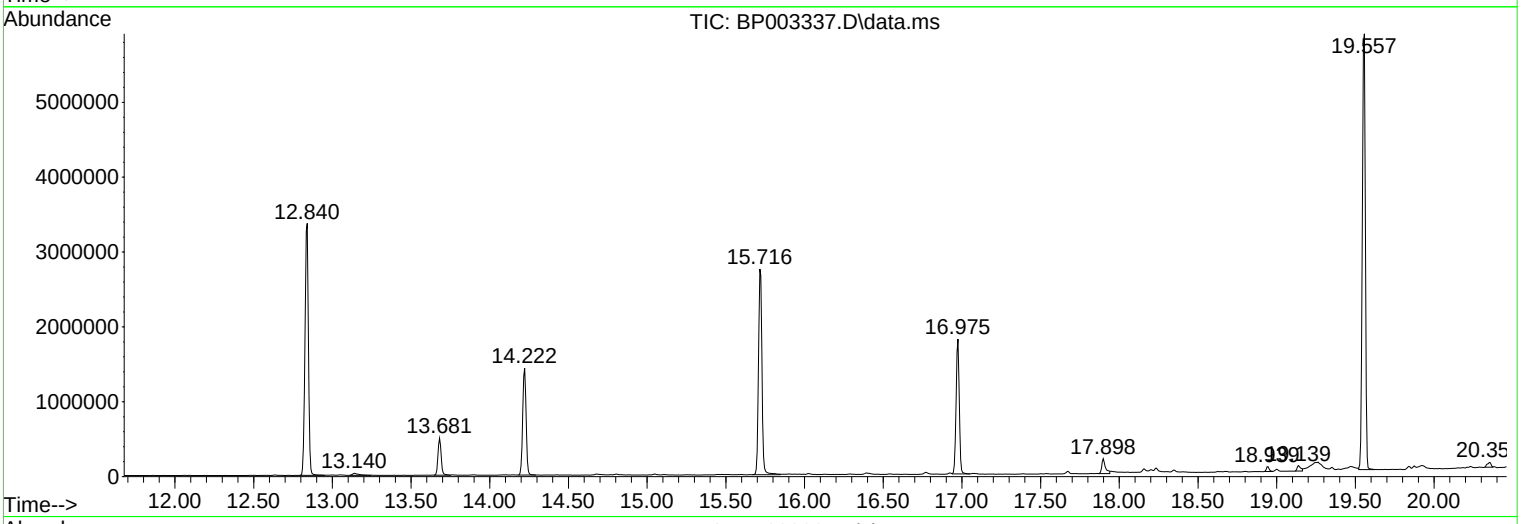
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

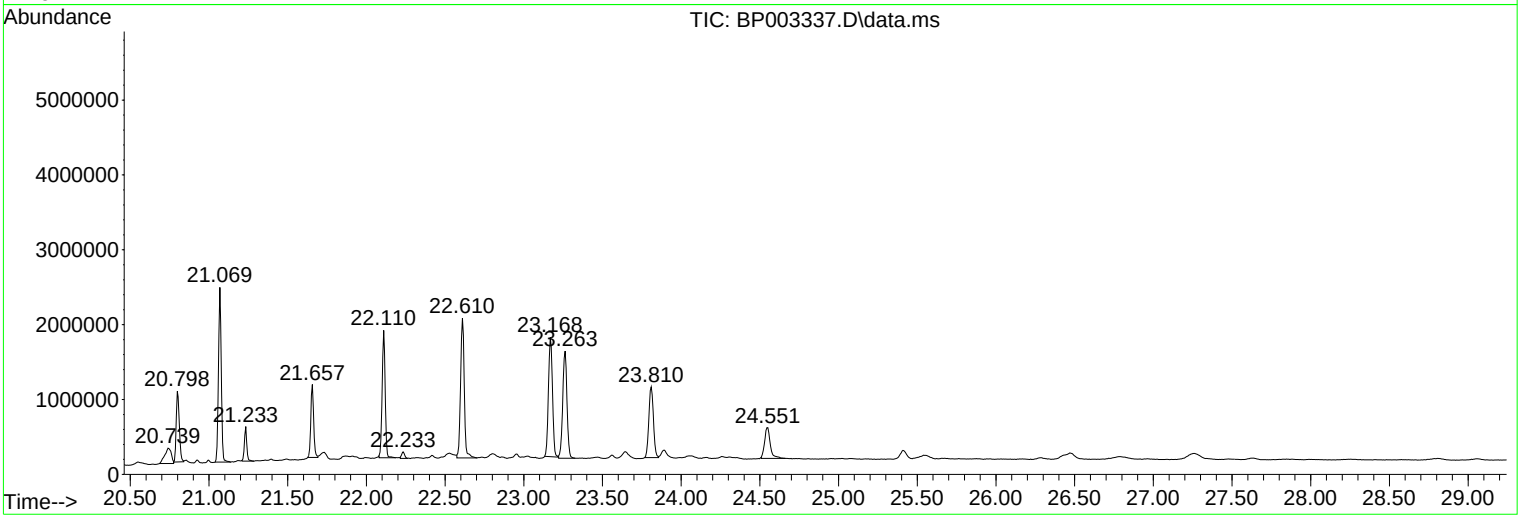
Instrument :
BNA_P
ClientSampleId :
RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
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Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

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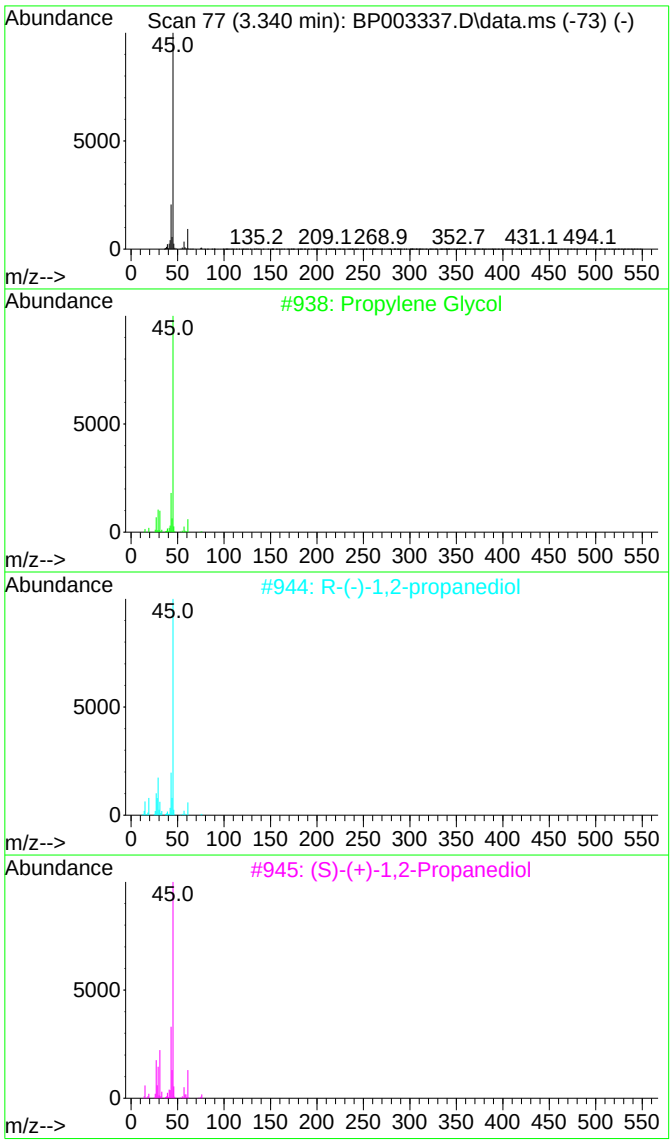
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

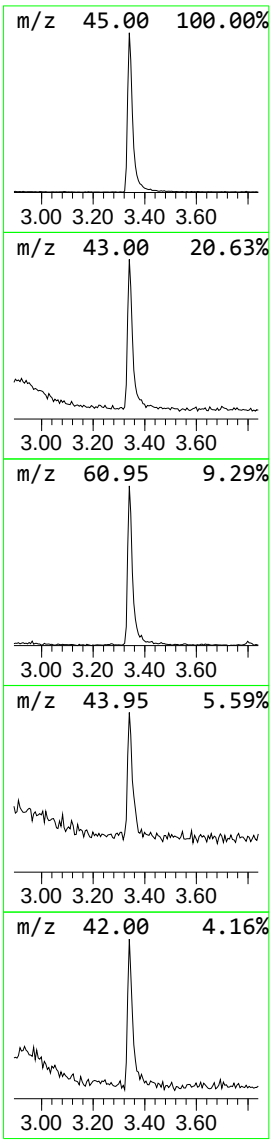
****

Peak Number 1 Propylene Glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.340	2.82 ng	138215	1,4-Dichlorobenzene-d4	7.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	L-Lactic acid	90	C3H6O3	000079-33-4	9
5	1-Propanol, 2-ethoxy-	104	C5H12O2	019089-47-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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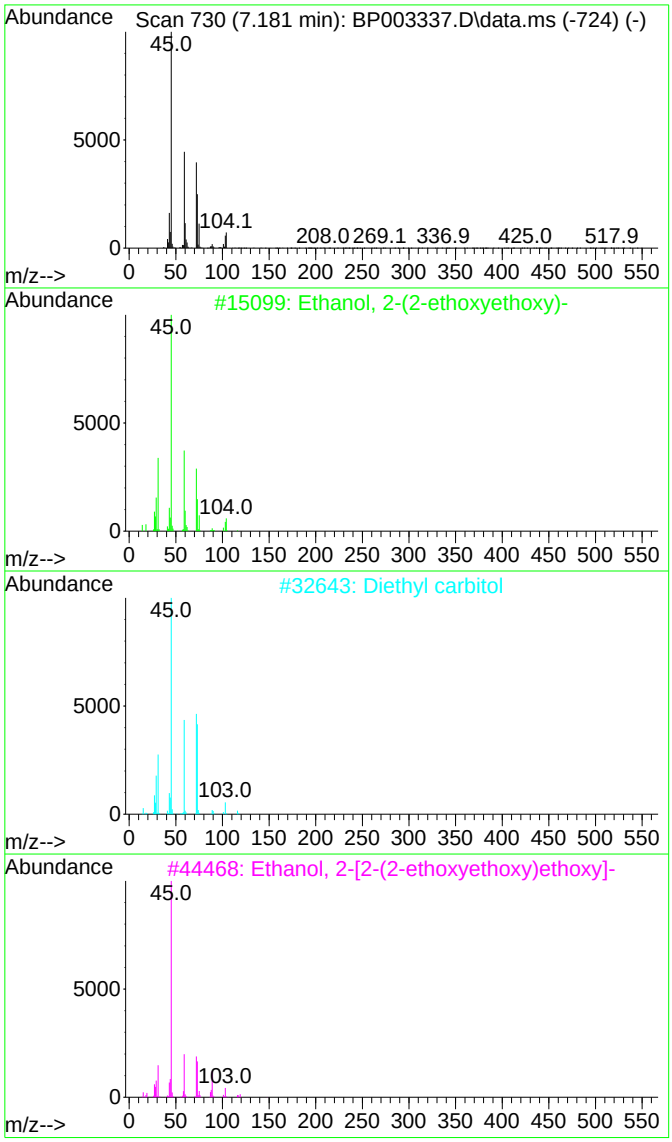
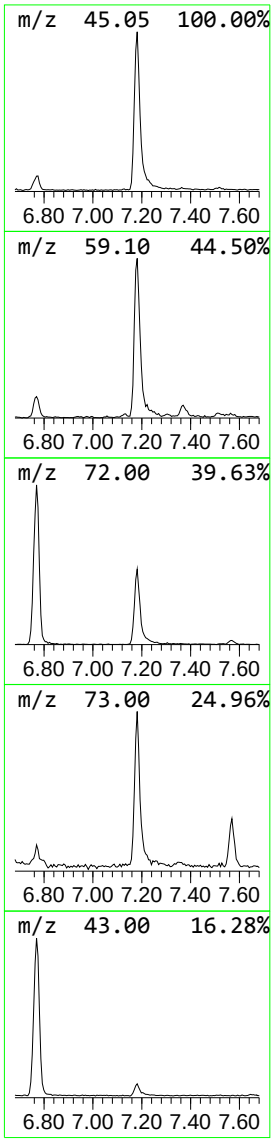
Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.181	2.14 ng	105078	1,4-Dichlorobenzene-d4	7.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	42
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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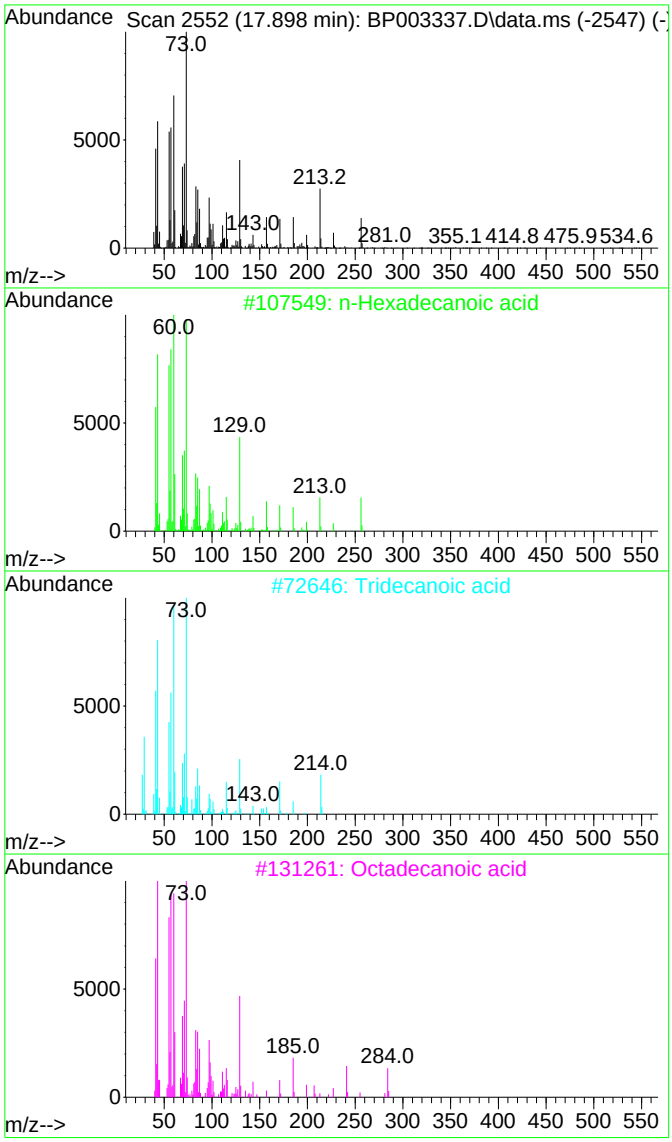
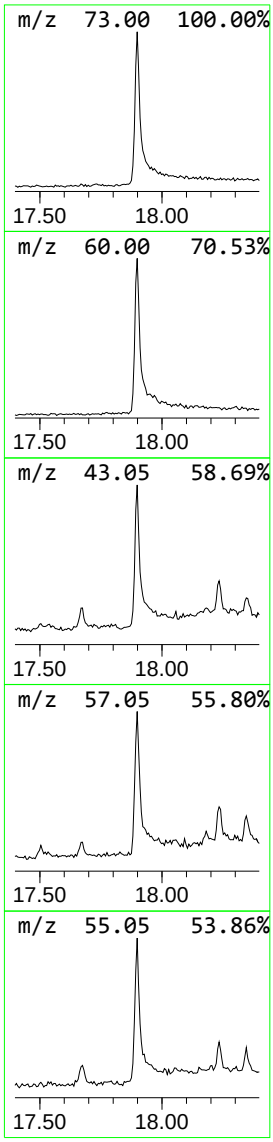
Peak Number 3 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.898	2.54 ng	320924	Phenanthrene-d10	16.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	74
4	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	60
5	Dodecanoic acid	200	C12H24O2	000143-07-7	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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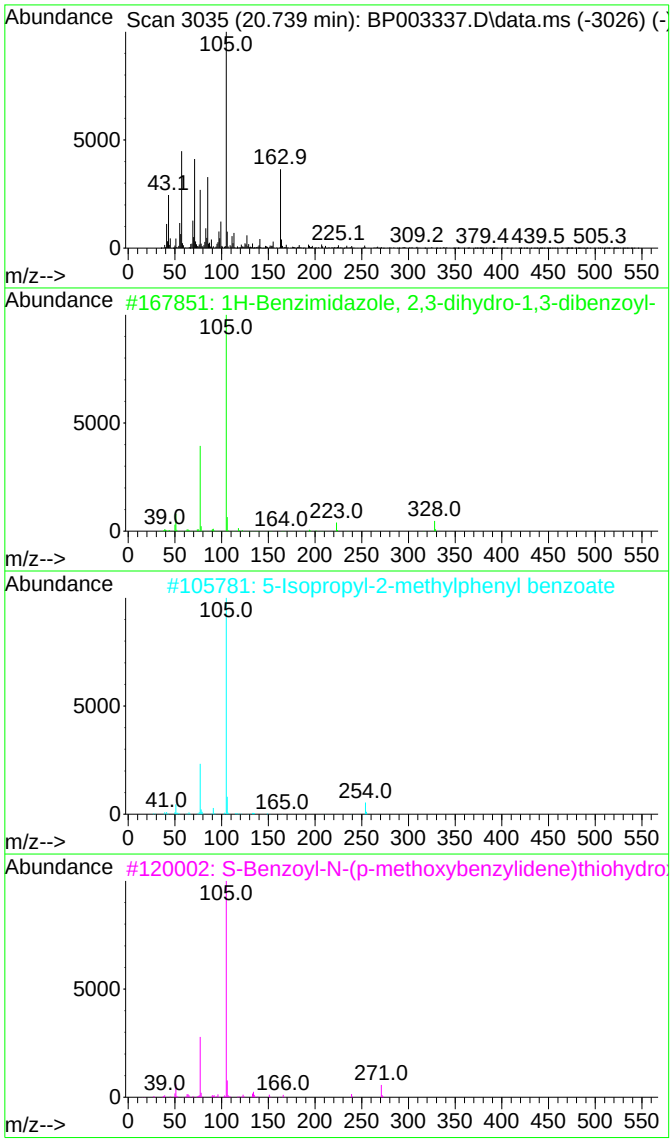
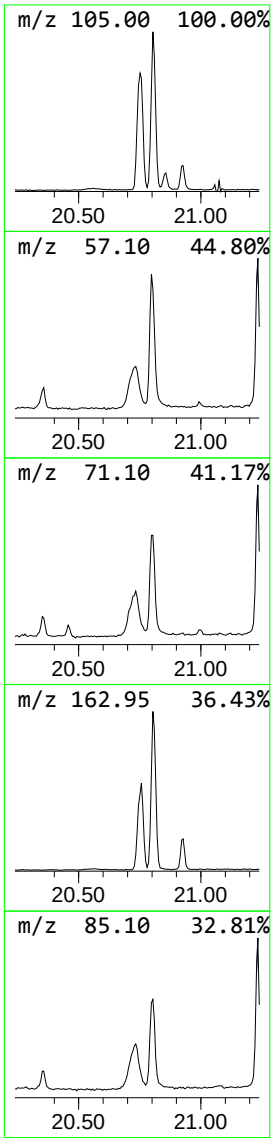
Peak Number 4 unknown20.73 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.739	4.04 ng	585840	Chrysene-d12	21.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2,3-dihydro-1,...	328	C21H16N2O2	1000262-54-9	14
2	5-Isopropyl-2-methylphenyl benzoate	254	C17H18O2	1000367-08-9	11
3	S-Benzoyl-N-(p-methoxybenzyliden...	271	C15H13NO2S	145198-44-3	10
4	2-Heptafluoropropyl-4-methylene-...	368	C15H11F7N2O	101948-90-7	10
5	9-Borabicyclo[3.3.1]nonane, 9-(b...	242	C15H19BO2	065212-33-1	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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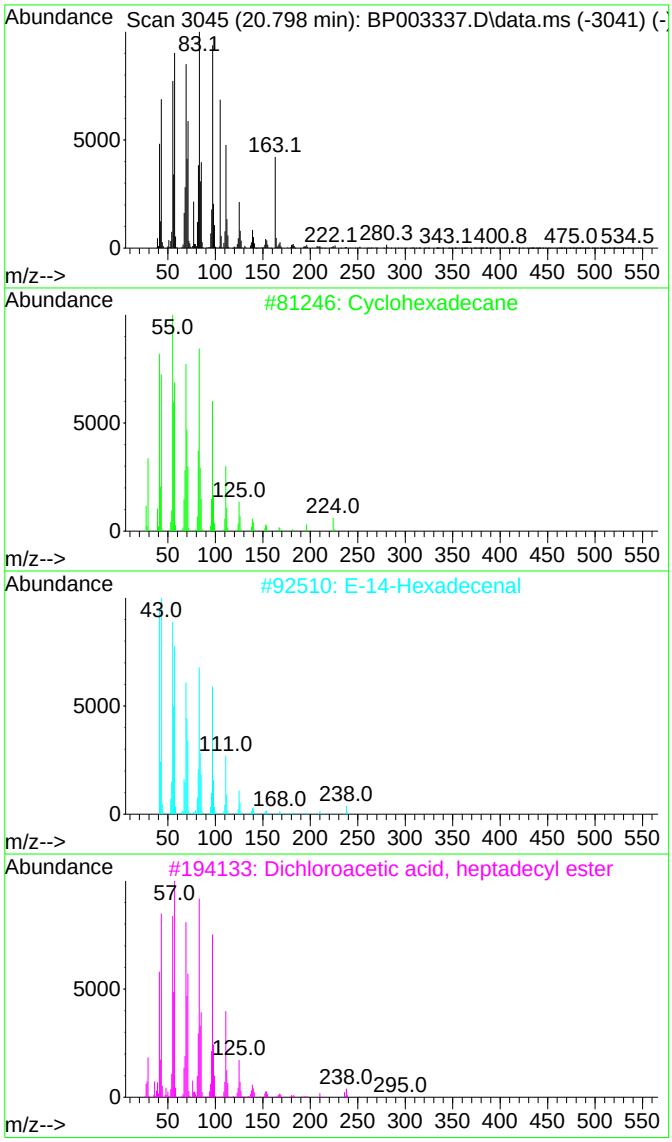
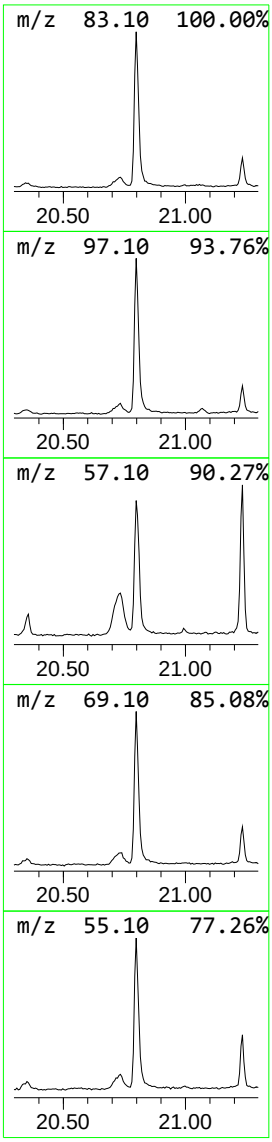
Peak Number 5 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.798	8.94 ng	1295990	Chrysene-d12	21.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	93
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	91
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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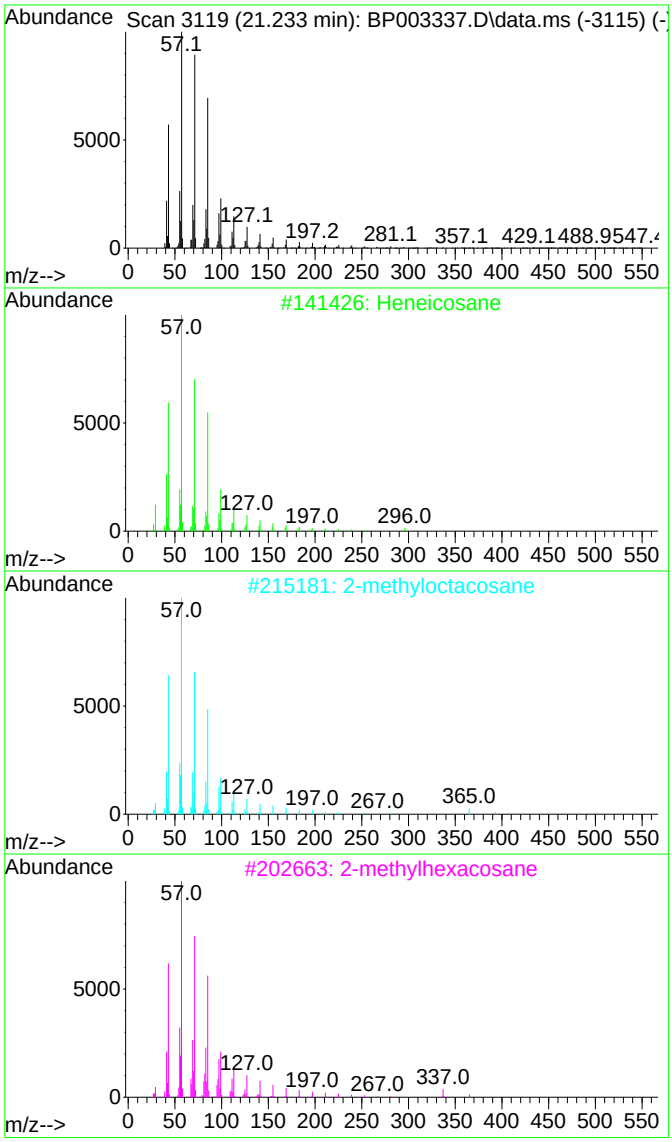
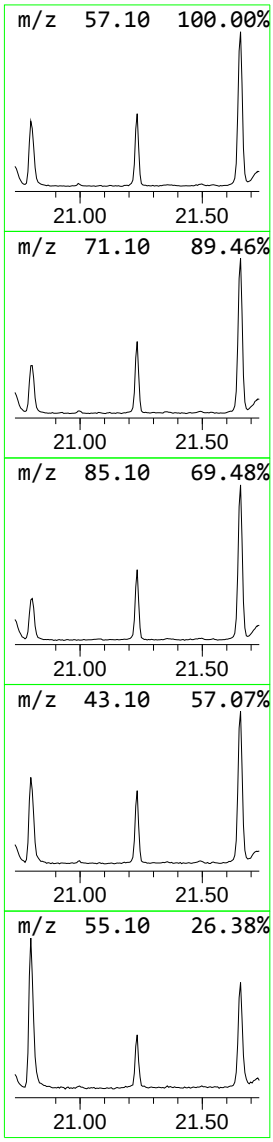
Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	3.35 ng	485992	Chrysene-d12	21.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	2-methylhexacosane	380	C27H56	1000376-72-7	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Eicosane	282	C20H42	000112-95-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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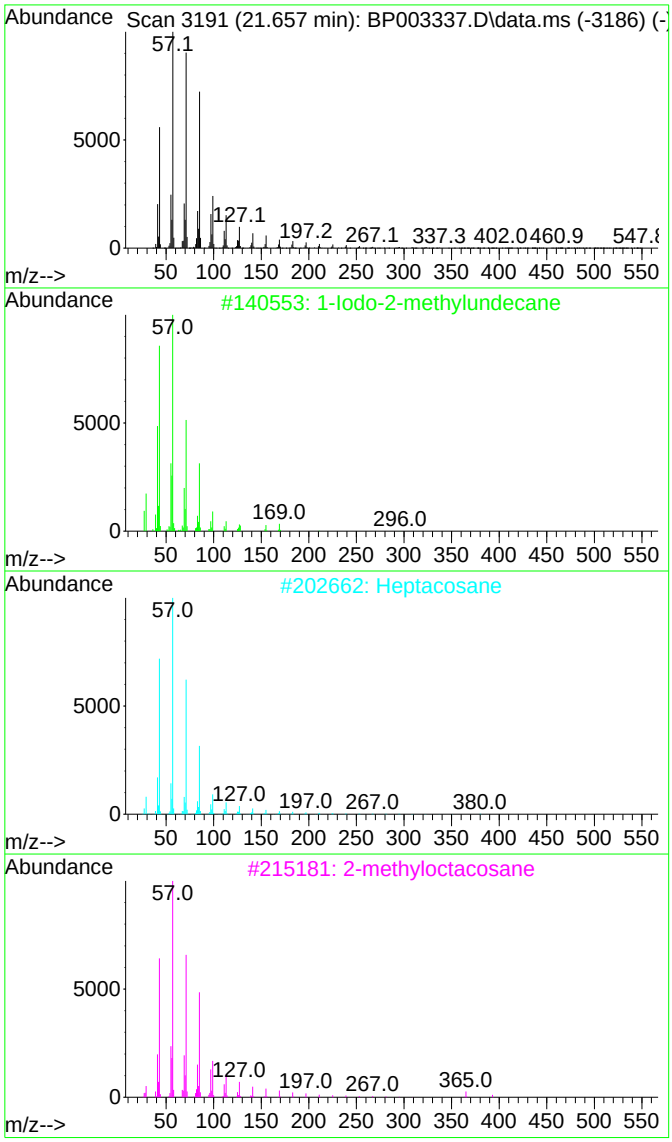
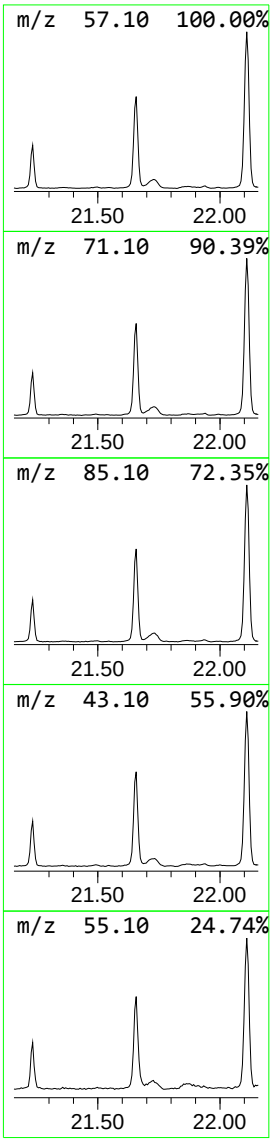
Peak Number 7 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.657	8.37 ng	1212930	Chrysene-d12	21.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Eicosane	282	C20H42	000112-95-8	91





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Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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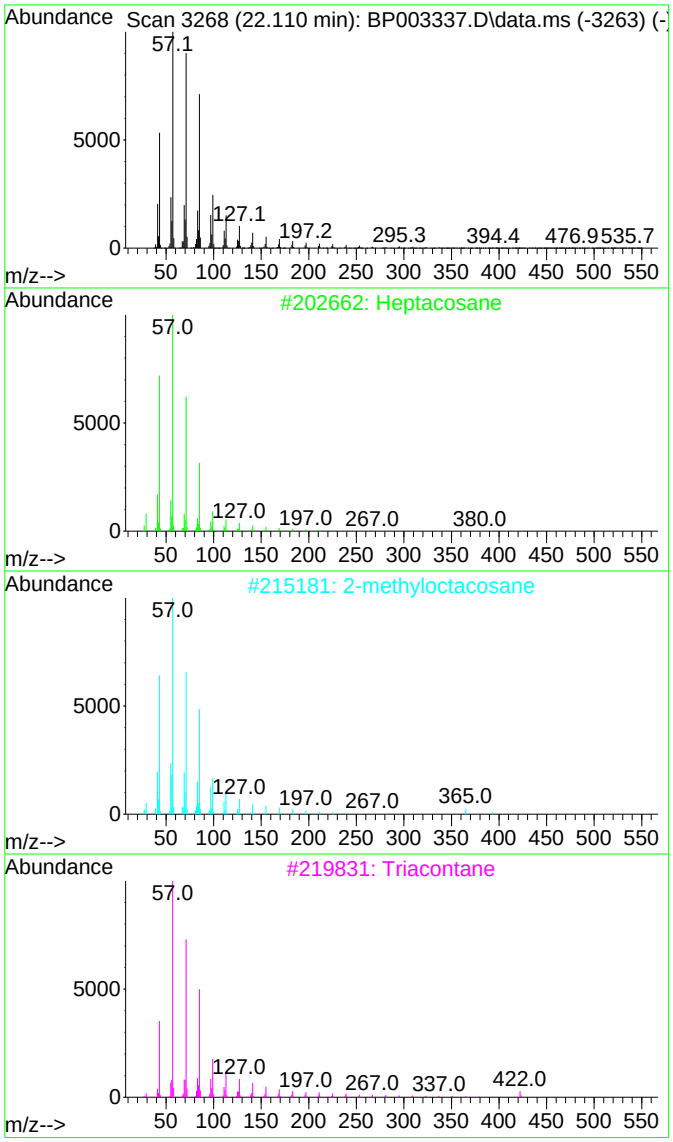
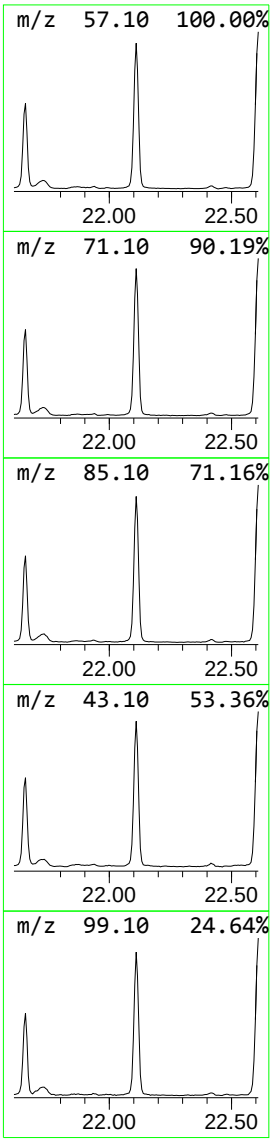
Peak Number 8 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.110	15.83 ng	2294720	Chrysene-d12	21.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RBR-59

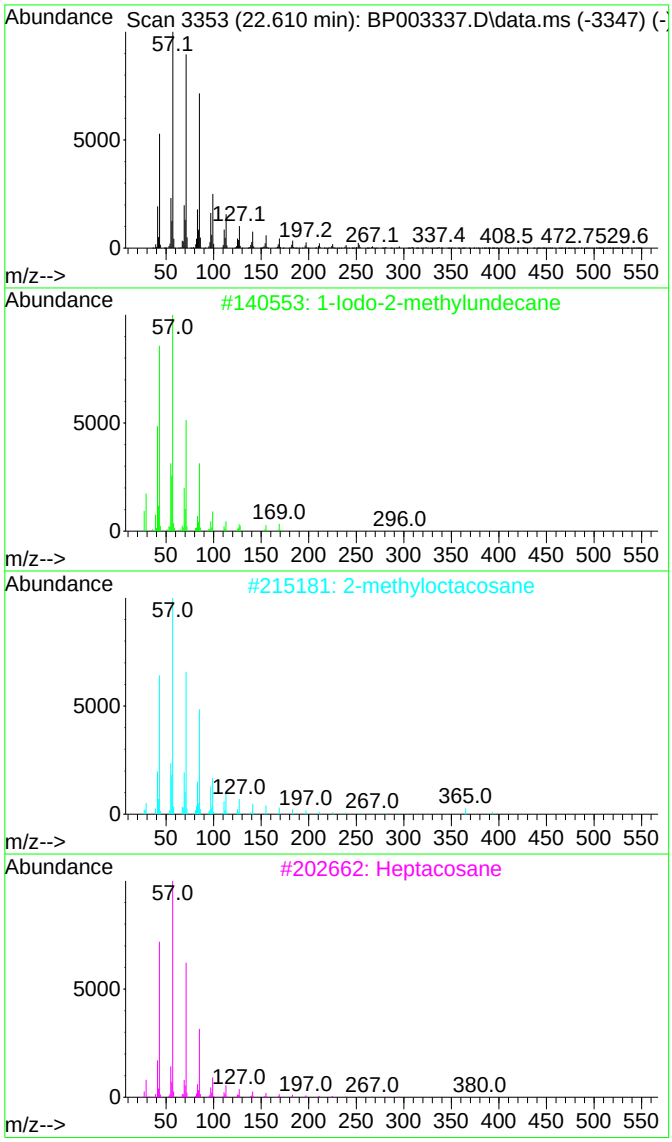
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

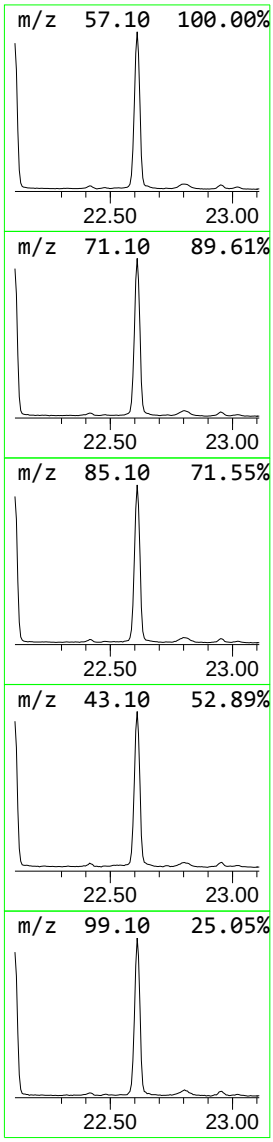
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Iodo-2-methylundecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.610	22.56 ng	3043470	Perylene-d12	23.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	94
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91





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Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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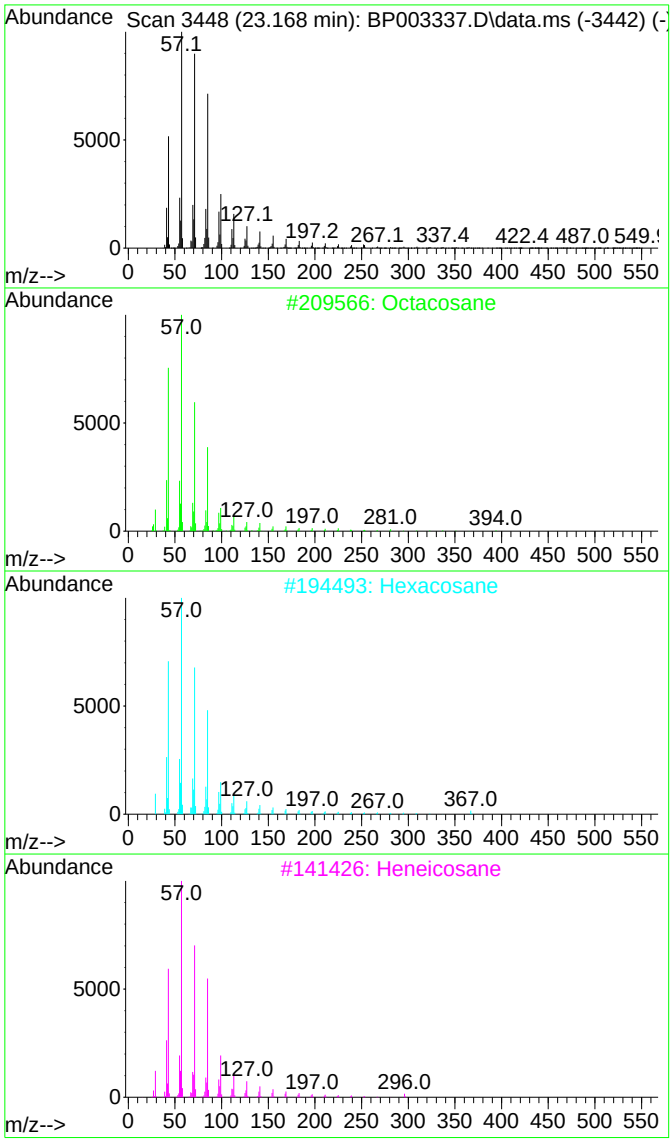
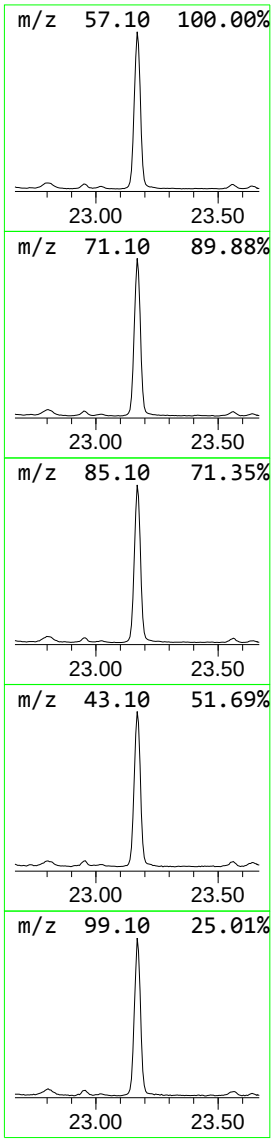
Peak Number 10 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.168	20.57 ng	2775530	Perylene-d12	23.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	94
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





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Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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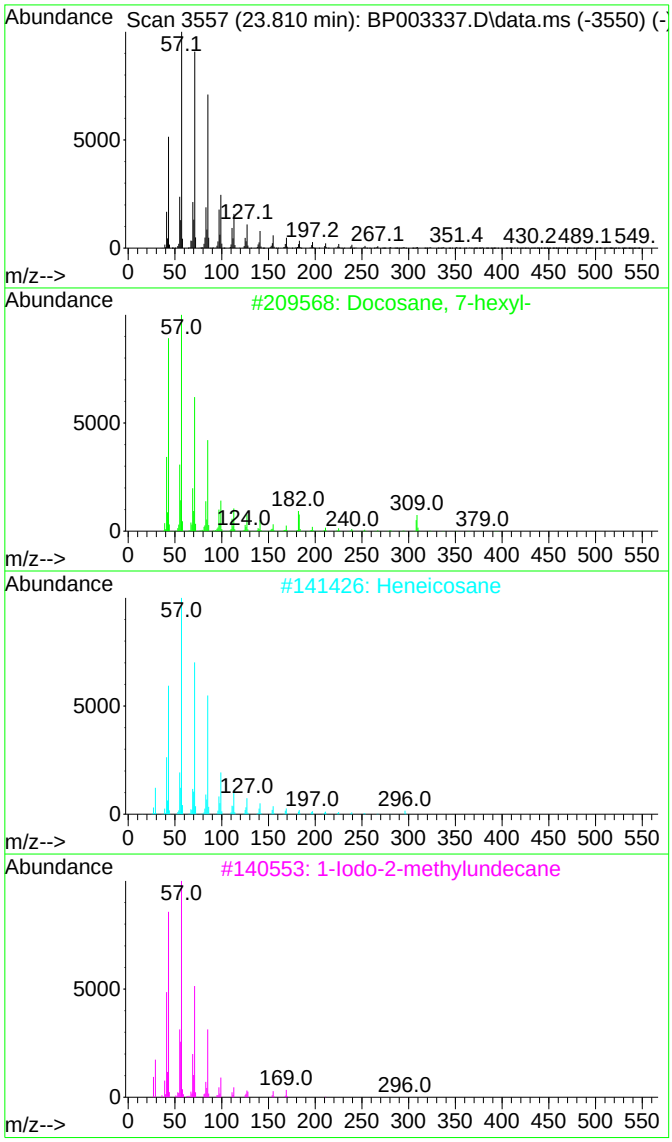
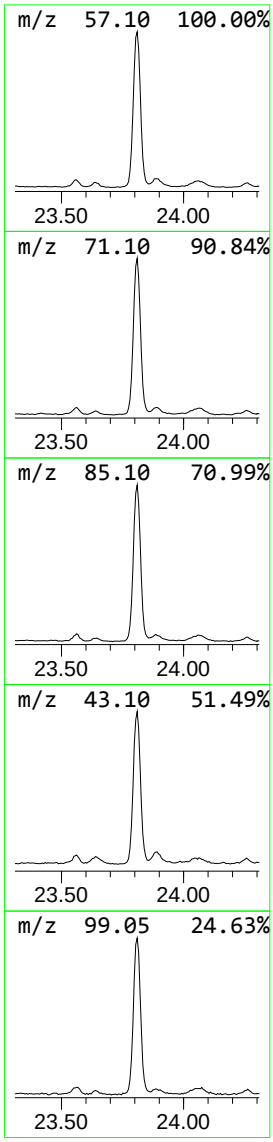
Peak Number 11 Docosane, 7-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.810	14.20 ng	1915380	Perylene-d12	23.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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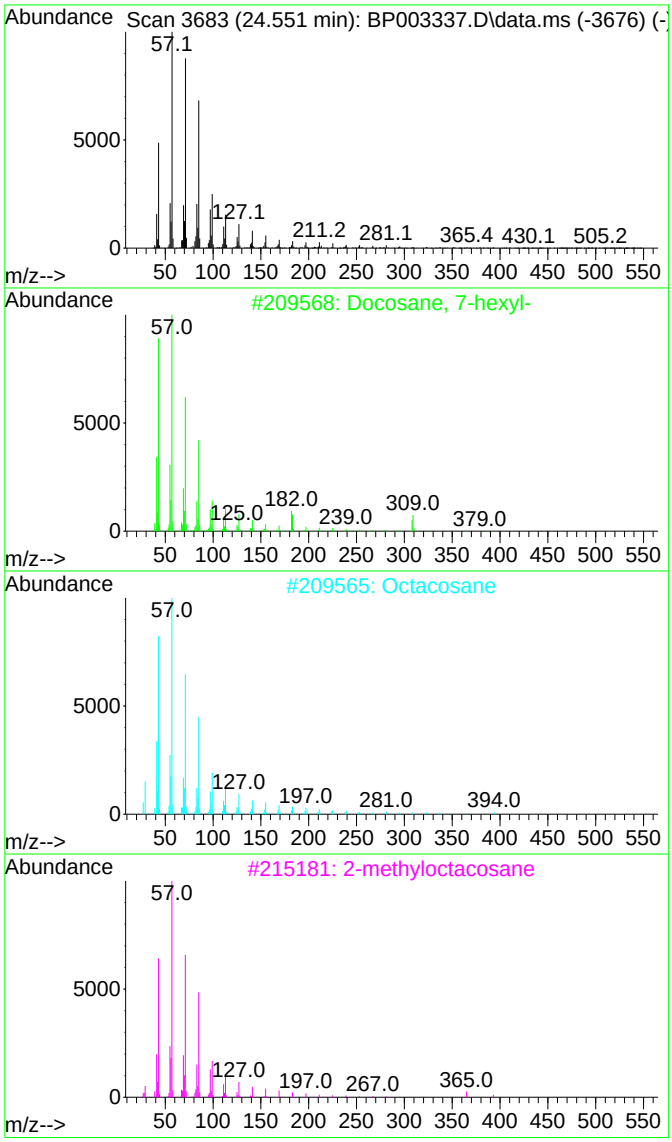
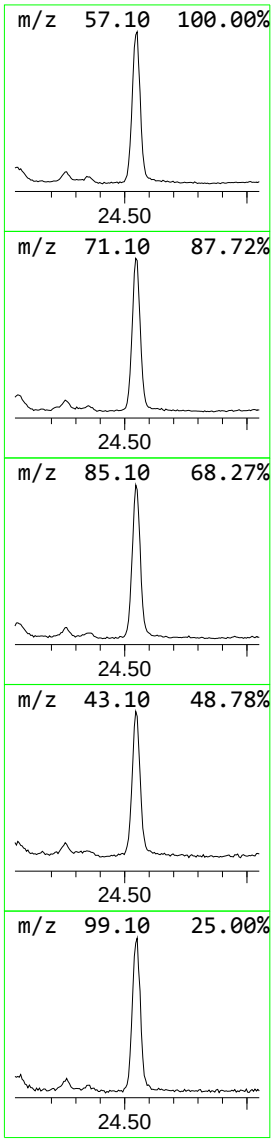
Peak Number 12 1-Heptadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.551	7.67 ng	1035410	Perylene-d12	23.262

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	1-Heptadecene	238	C17H34	006765-39-5	91
5	2-methyltetracosane	352	C25H52	1000376-72-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003337.D
Acq On : 22 Sep 2020 14:06
Operator : CG/JU
Sample : L4100-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-59

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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
Propylene Glycol	3.340	2.8	ng	138215	1	7.569	981653	20.0
Ethanol, 2-(2-e...	7.181	2.1	ng	105078	1	7.569	981653	20.0
n-Hexadecanoic ...	17.898	2.5	ng	320924	4	16.975	2523080	20.0
unknown20.73	20.739	4.0	ng	585840	5	21.069	2899120	20.0
Cyclohexadecane	20.798	8.9	ng	1295990	5	21.069	2899120	20.0
Heneicosane	21.233	3.4	ng	485992	5	21.069	2899120	20.0
2-methyloctacosane	21.657	8.4	ng	1212930	5	21.069	2899120	20.0
Heptacosane	22.110	15.8	ng	2294720	5	21.069	2899120	20.0
1-Iodo-2-methyl...	22.610	22.6	ng	3043470	6	23.262	2698600	20.0
Octacosane	23.168	20.6	ng	2775530	6	23.262	2698600	20.0
Docosane, 7-hexyl-	23.810	14.2	ng	1915380	6	23.262	2698600	20.0
1-Heptadecene	24.551	7.7	ng	1035410	6	23.262	2698600	20.0