LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003597.D
Acq On : 09 Oct 2020 17:13
Operator : CG/JU
Sample : L4318-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 214

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: BP003597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.611	289	293	302	rBV	47969	70603	3.24%	0.637%
2	5.099	370	376	394	rBV	436483	753392	34.61%	6.795%
3	6.693	641	647	678	rBV	386661	759475	34.89%	6.850%
4	7.475	774	780	793	rBV	136251	232418	10.68%	2.096%
5	8.634	970	977	1000	rBV	288095	553434	25.43%	4.992%
6	10.251	1244	1252	1275	rBV	159070	313933	14.42%	2.832%
7	12.751	1670	1677	1692	rBV	898855	1375374	63.19%	12.405%
8	13.051	1722	1728	1739	rVB	35138	57263	2.63%	0.516%
9	13.604	1817	1822	1837	rBV	102751	176628	8.11%	1.593%
10	14.139	1904	1913	1924	rBV	278947	428453	19.68%	3.865%
11	15.645	2163	2169	2179	rBV	683411	1047835	48.14%	9.451%
12	15.910	2212	2214	2218	rVB	30022	35227	1.62%	0.318%
13	16.898	2377	2382	2392	rBV	329924	499308	22.94%	4.504%
14	19.486	2817	2822	2832	rVB	1753557	2176631	100.00%	19.633%
15	20.727	3029	3033	3043	rBV	260222	352140	16.18%	3.176%
16	21.010	3076	3081	3090	rBV	483899	633404	29.10%	5.713%
17	21.592	3176	3180	3189	rVB	202226	310286	14.26%	2.799%
18	22.239	3288	3290	3295	rVB2	34613	40345	1.85%	0.364%
19	22.510	3332	3336	3340	rBV	88368	124194	5.71%	1.120%
20	22.557	3340	3344	3354	rVB	85619	153551	7.05%	1.385%
21	23.174	3443	3449	3461	rVB	360419	705707	32.42%	6.365%
22	23.680	3531	3535	3541	rVB	93453	161758	7.43%	1.459%
23	23.762	3545	3549	3560	rVB	55948	125470	5.76%	1.132%

Sum of corrected areas: 11086829

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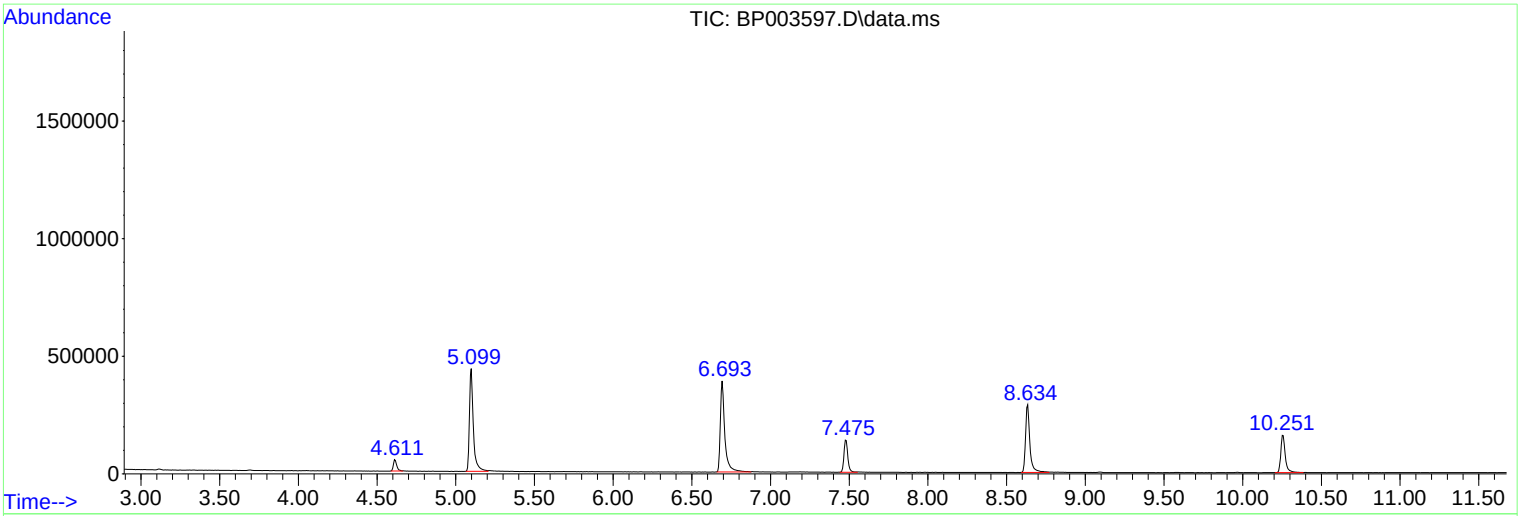
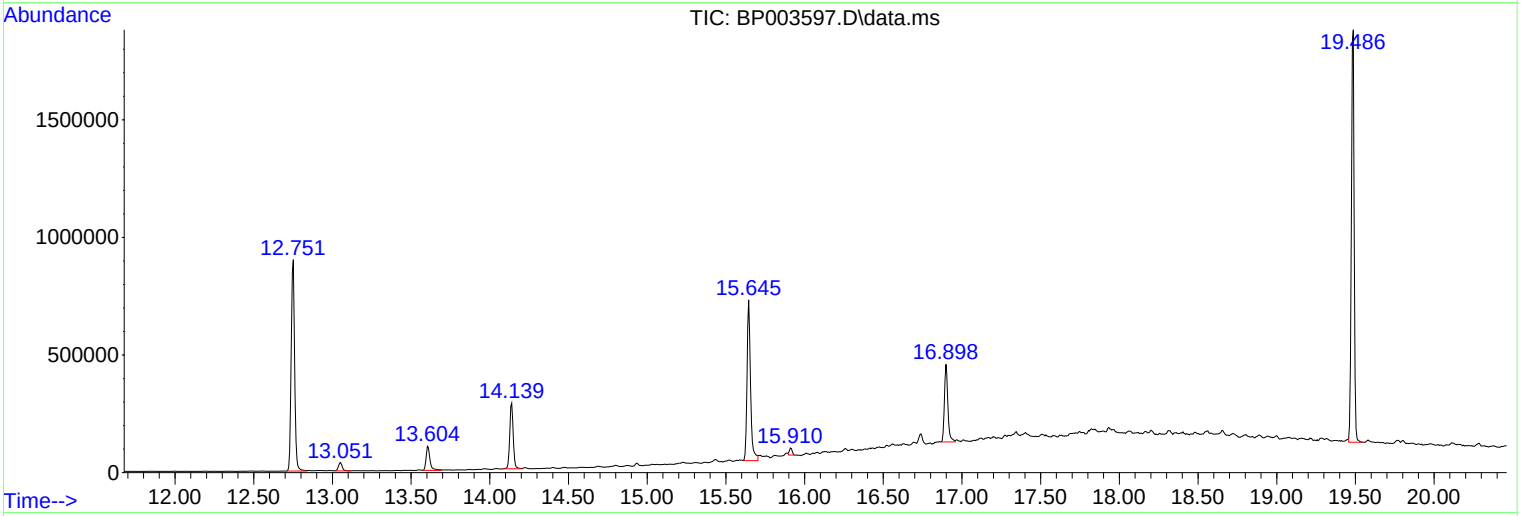
Sample : L4318-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

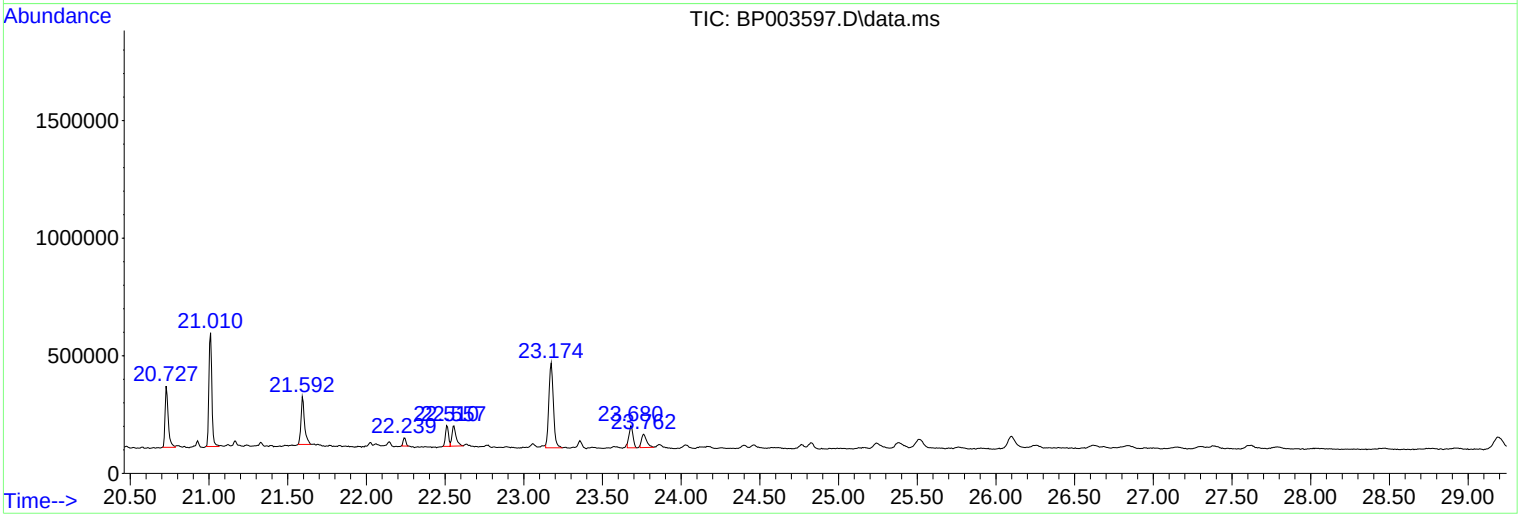
Instrument :
BNA_P
ClientSampleId :
214

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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Data File : BP003597.D
Acq On : 09 Oct 2020 17:13
Operator : CG/JU
Sample : L4318-01
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ClientSampleId :
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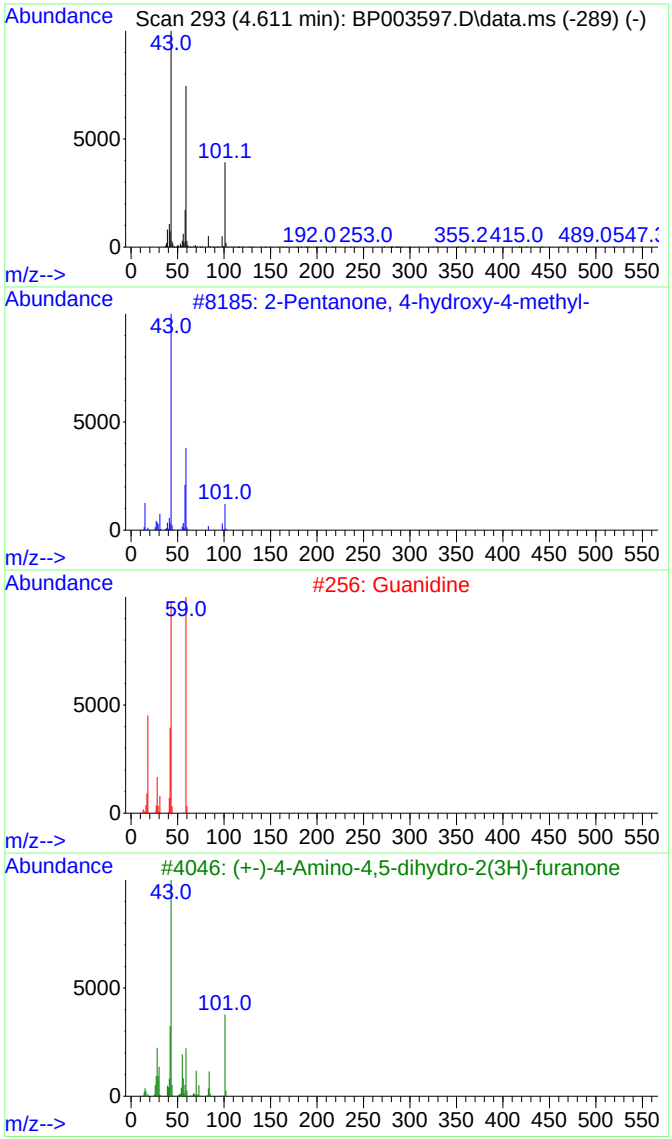
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

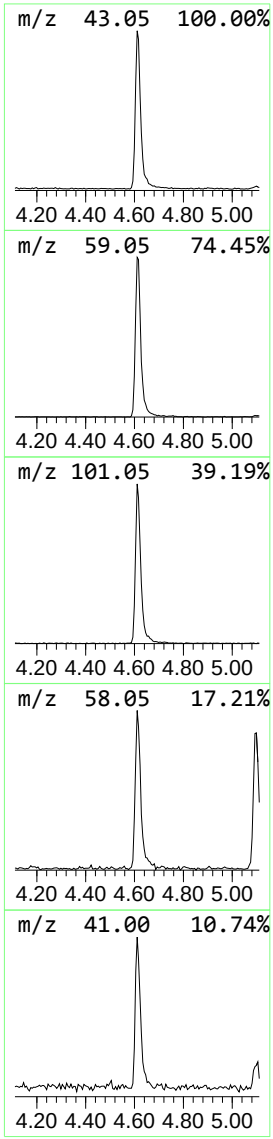
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.611	6.08 ng	70603	1,4-Dichlorobenzene-d4	7.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23





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Data File : BP003597.D
Acq On : 09 Oct 2020 17:13
Operator : CG/JU
Sample : L4318-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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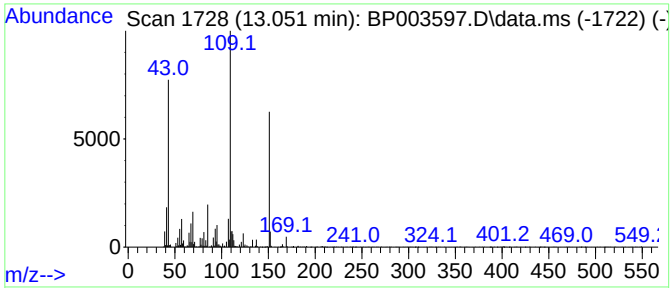
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

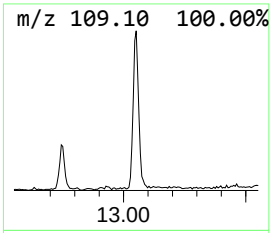
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

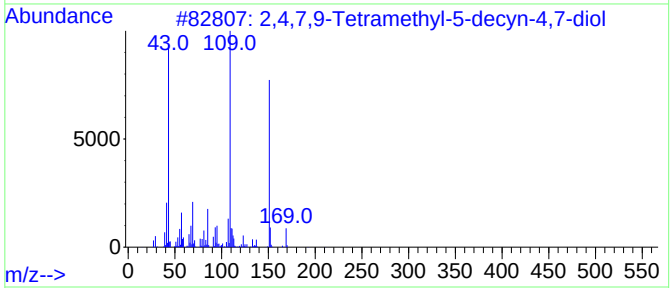
****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

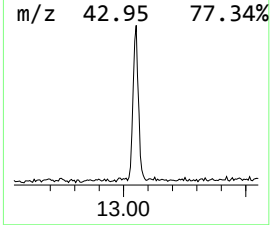
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.051	2.67 ng	57263	Acenaphthene-d10	14.139

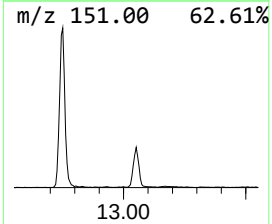
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	64
3	Tiocarlide	400	C23H32N2O2S	000910-86-1	53
4	Metacetamol	151	C8H9NO2	000621-42-1	53
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	50

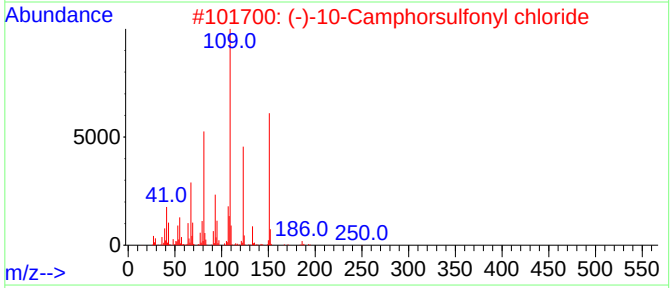


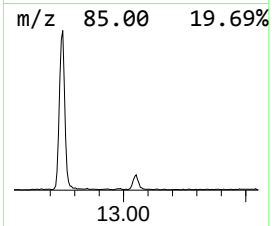


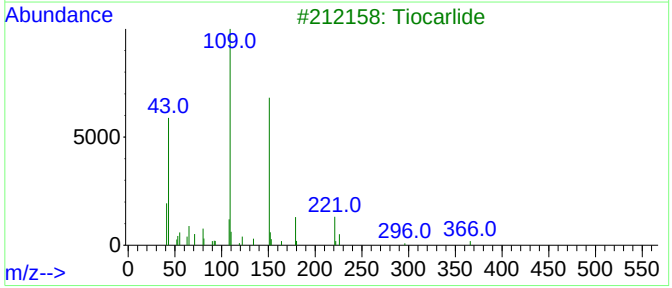


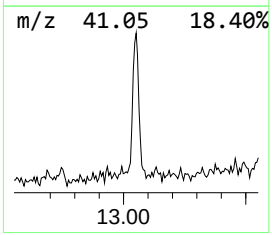












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Data File : BP003597.D
Acq On : 09 Oct 2020 17:13
Operator : CG/JU
Sample : L4318-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 214

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

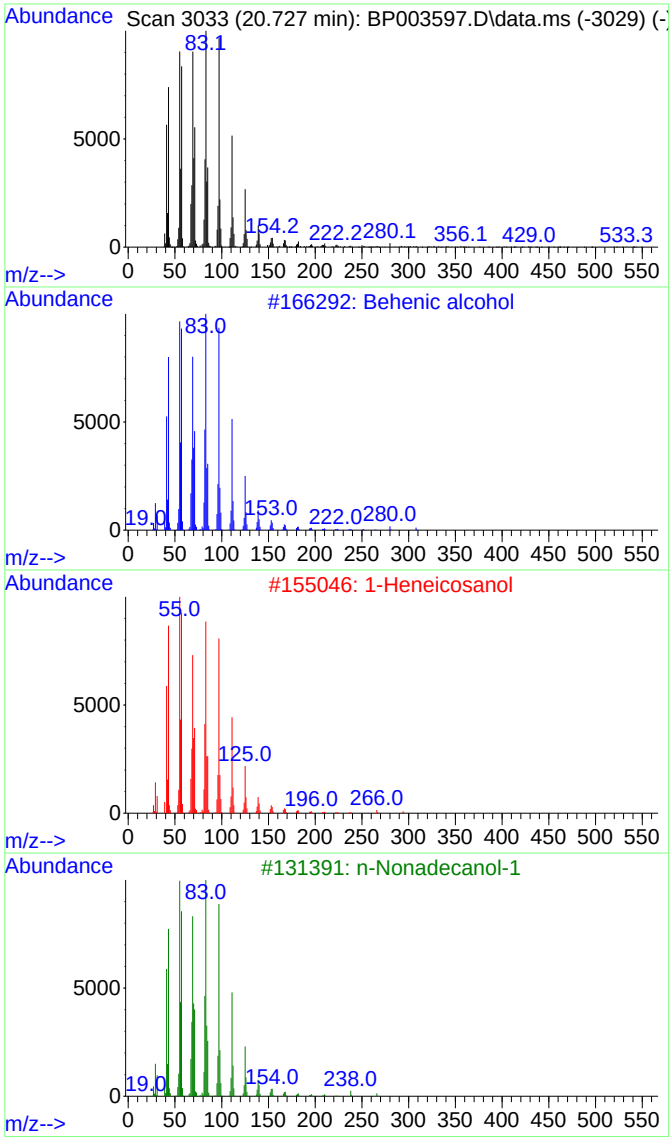
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

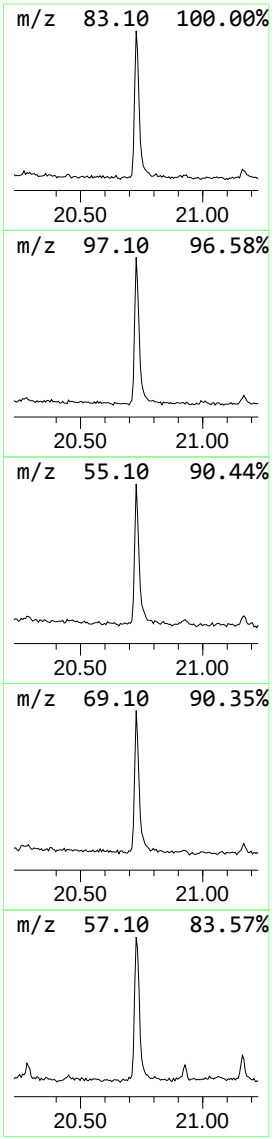
****

Peak Number 3 Behenic alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.727	11.12 ng	352140	Chrysene-d12	21.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	93





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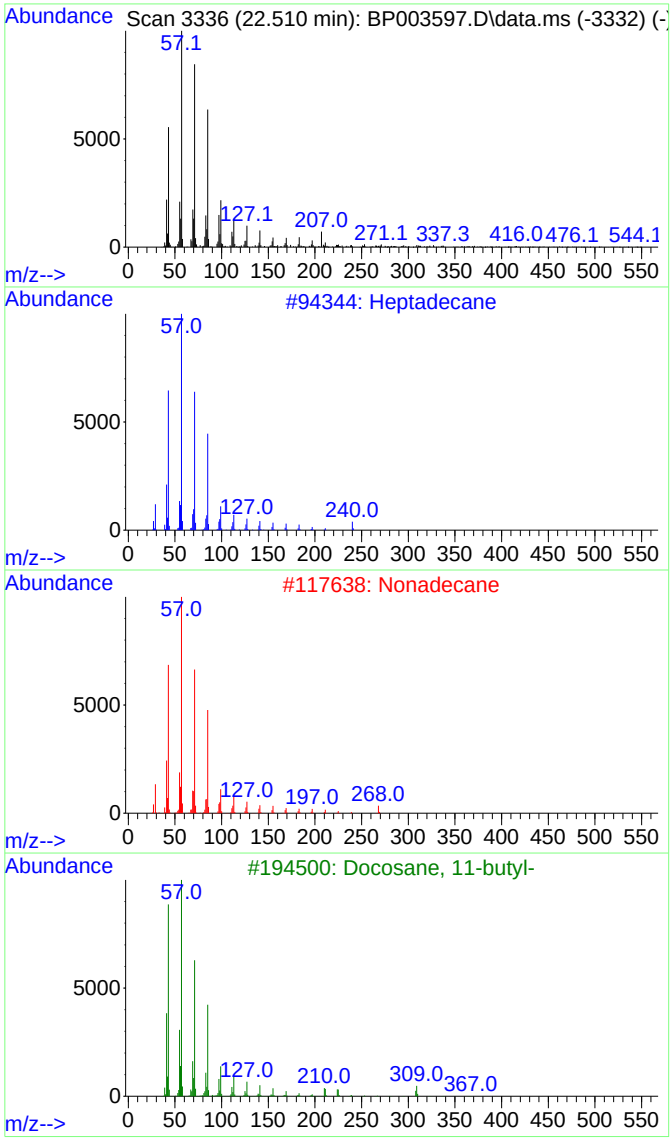
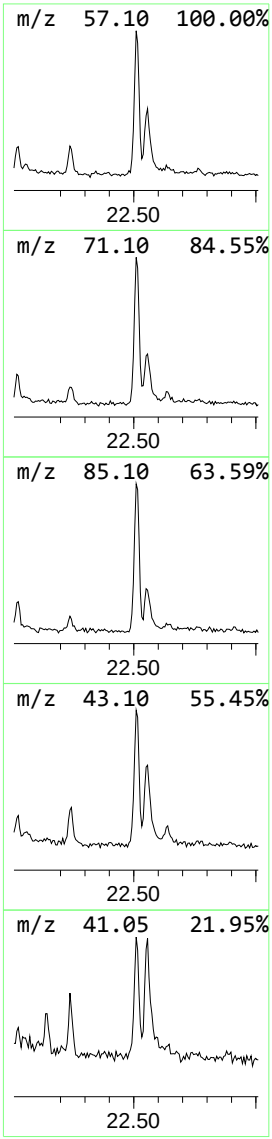
****

Peak Number 5 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.510	3.52 ng	124194	Perylene-d12	23.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Nonadecane	268	C19H40	000629-92-5	94
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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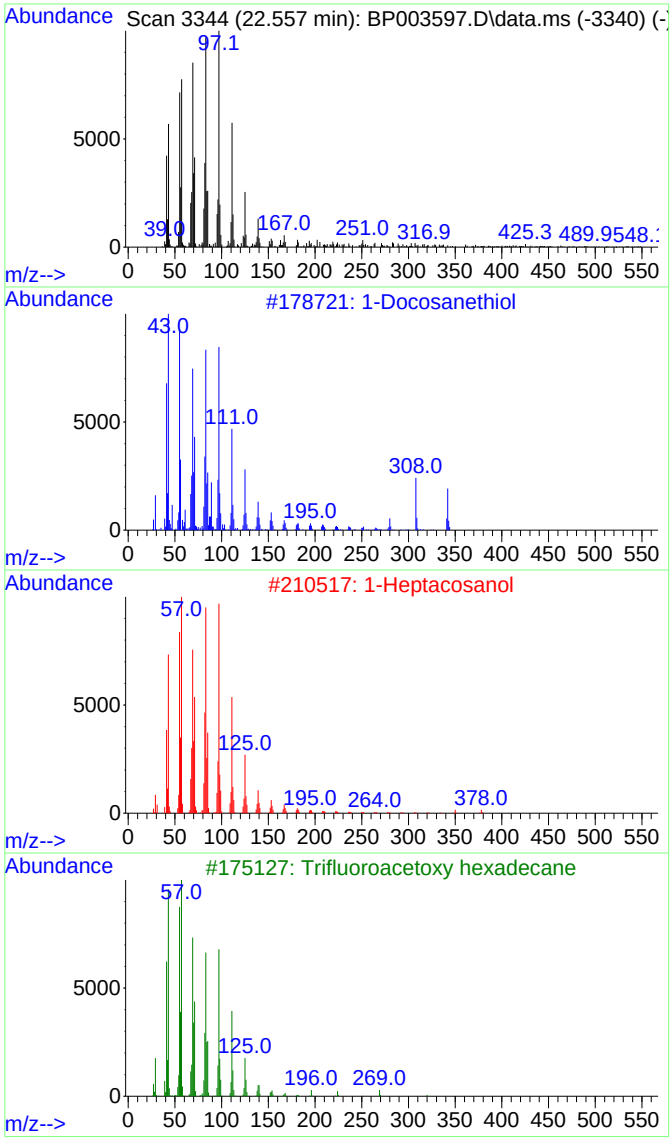
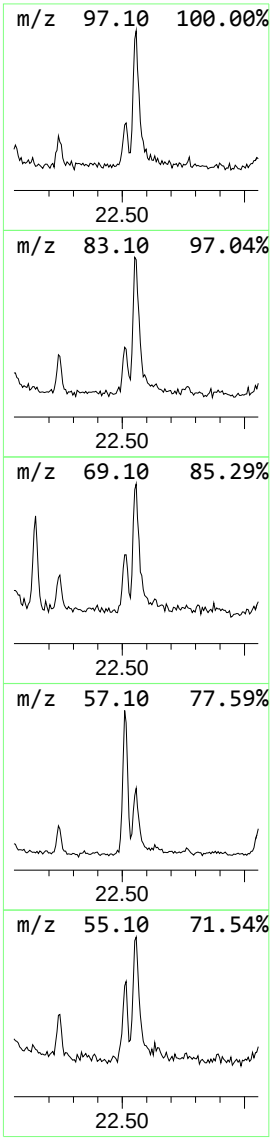
****

Peak Number 6 1-Docosanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.557	4.35 ng	153551	Perylene-d12	23.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanethiol	342	C22H46S	007773-83-3	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	83
5	1-Heneicosanol	312	C21H44O	015594-90-8	81





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Sample : L4318-01
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Instrument : BNA_P
ClientSampleId : 214

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

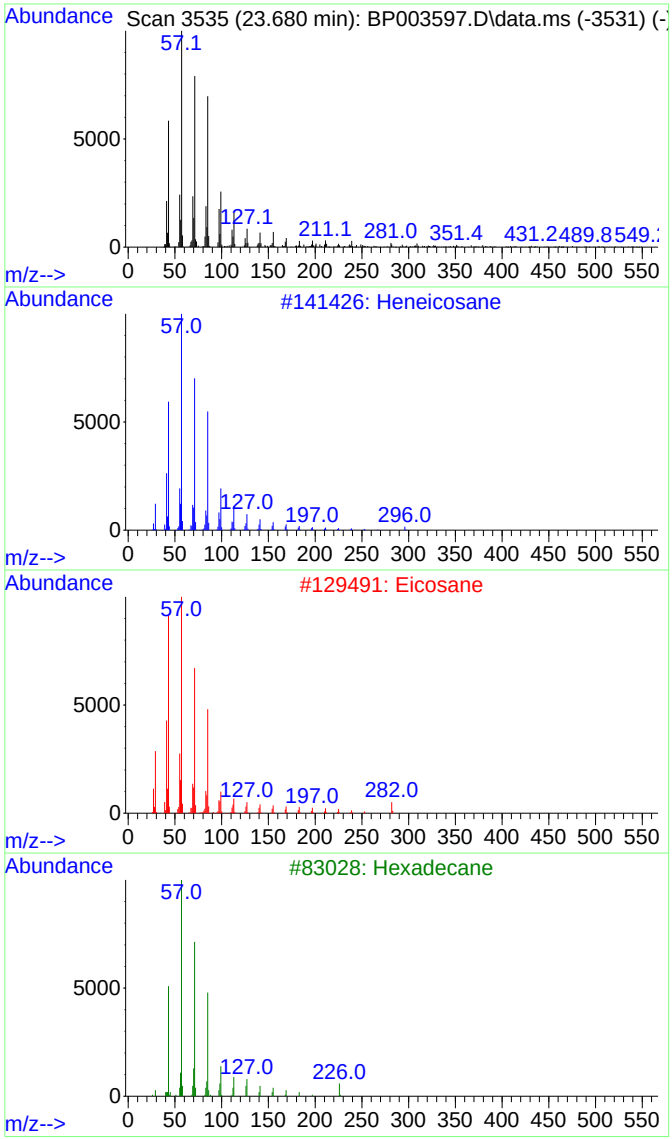
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

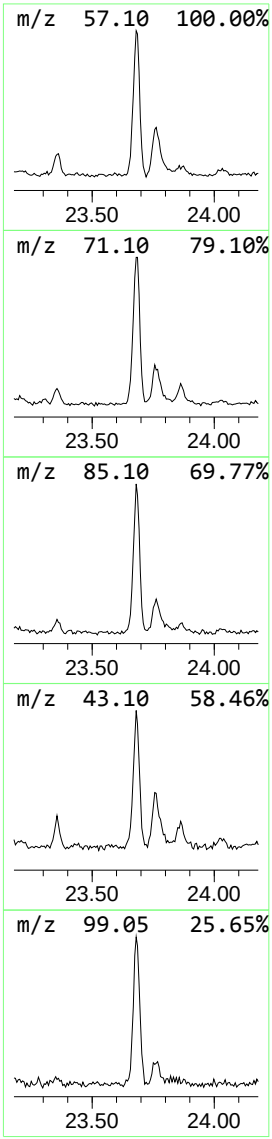
****

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.680	4.58 ng	161758	Perylene-d12	23.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Eicosane	282	C20H42	000112-95-8	95
3	Hexadecane	226	C16H34	000544-76-3	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Octacosane	394	C28H58	000630-02-4	91





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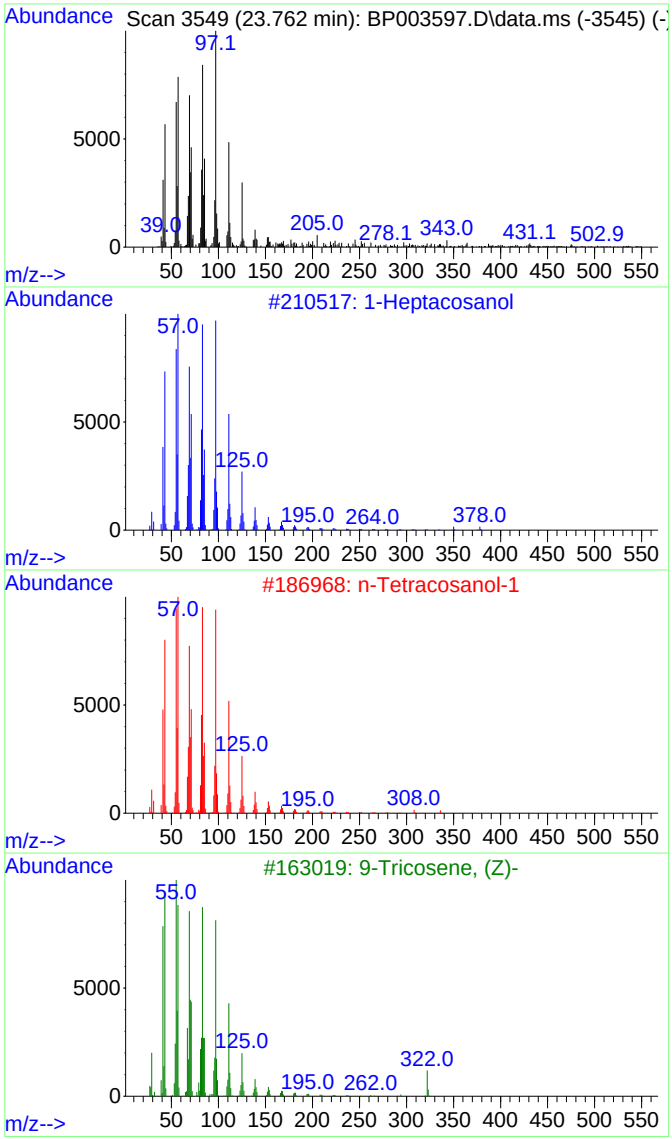
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

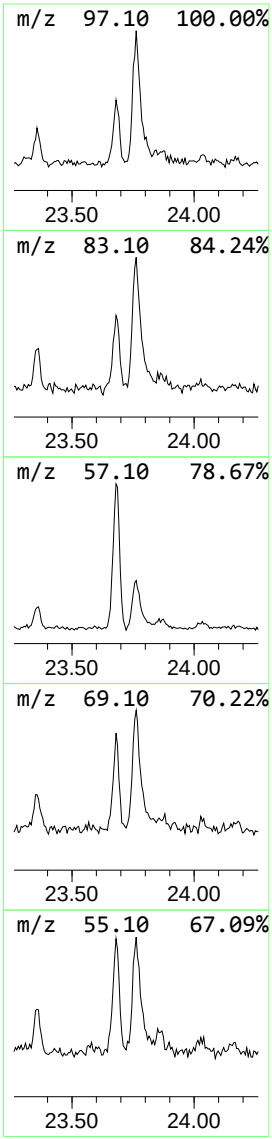
****

Peak Number 8 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.762	3.56 ng	125470	Perylene-d12	23.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
4	Cyclooctacosane	392	C28H56	000297-24-5	90
5	Cyclotetracosane	336	C24H48	000297-03-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003597.D
Acq On : 09 Oct 2020 17:13
Operator : CG/JU
Sample : L4318-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
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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
2-Pentanone, 4-...	4.611	6.1	ng	70603	1	7.481	232418	20.0
2,4,7,9-Tetrame...	13.051	2.7	ng	57263	3	14.139	428453	20.0
Behenic alcohol	20.727	11.1	ng	352140	5	21.010	633404	20.0
Heptadecane	22.510	3.5	ng	124194	6	23.174	705707	20.0
1-Docosanethiol	22.557	4.3	ng	153551	6	23.174	705707	20.0
Heneicosane	23.680	4.6	ng	161758	6	23.174	705707	20.0
1-Heptacosanol	23.762	3.6	ng	125470	6	23.174	705707	20.0