LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019685.D
Acq On : 13 Feb 2024 19:24
Operator : MA/JU
Sample : P1446-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT3475

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-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019685.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.628	88	92	100	rBV	38577	59472	1.18%	0.292%
2	4.417	219	226	232	rBV	123940	173852	3.45%	0.855%
3	5.022	323	329	339	rVB	396343	580700	11.53%	2.855%
4	5.475	399	406	416	rBV	845434	1272378	25.27%	6.255%
5	7.075	666	678	691	rBV	1069419	1757756	34.91%	8.641%
6	7.905	812	819	826	rBV	239812	397973	7.90%	1.956%
7	9.069	1009	1017	1028	rBV	710158	1251513	24.86%	6.152%
8	10.705	1287	1295	1303	rBV	293145	525671	10.44%	2.584%
9	13.163	1701	1713	1735	rBV	1941811	3083065	61.23%	15.155%
10	14.534	1940	1946	1956	rBV	438517	712491	14.15%	3.502%
11	14.763	1976	1985	1997	rVB2	174763	410506	8.15%	2.018%
12	16.028	2194	2200	2220	rBV	777446	1267835	25.18%	6.232%
13	17.292	2408	2415	2424	rBV	597779	921038	18.29%	4.528%
14	18.187	2563	2567	2577	rBV	88831	134677	2.67%	0.662%
15	19.863	2846	2852	2857	rBV	4038881	5034881	100.00%	24.750%
16	20.616	2976	2980	2985	rBV	238082	283712	5.63%	1.395%
17	21.110	3060	3064	3069	rBV	224086	306203	6.08%	1.505%
18	21.386	3106	3111	3117	rVB	753466	1022223	20.30%	5.025%
19	23.804	3516	3522	3532	rVB	529544	1146995	22.78%	5.638%

Sum of corrected areas: 20342941

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019685.D
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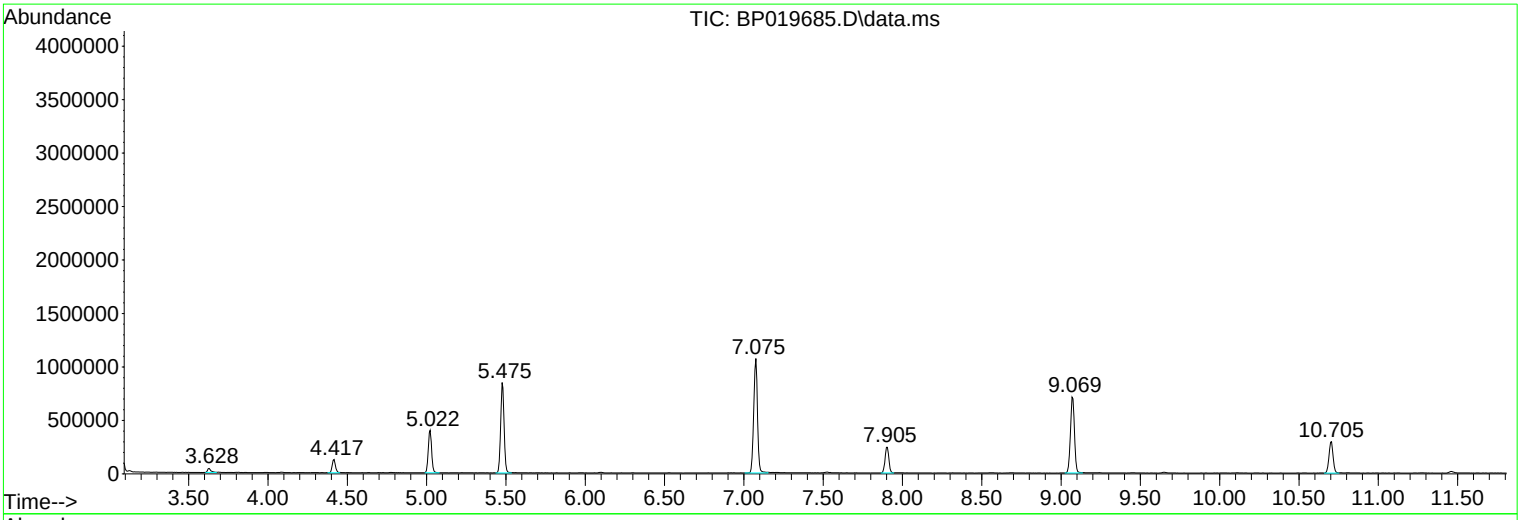
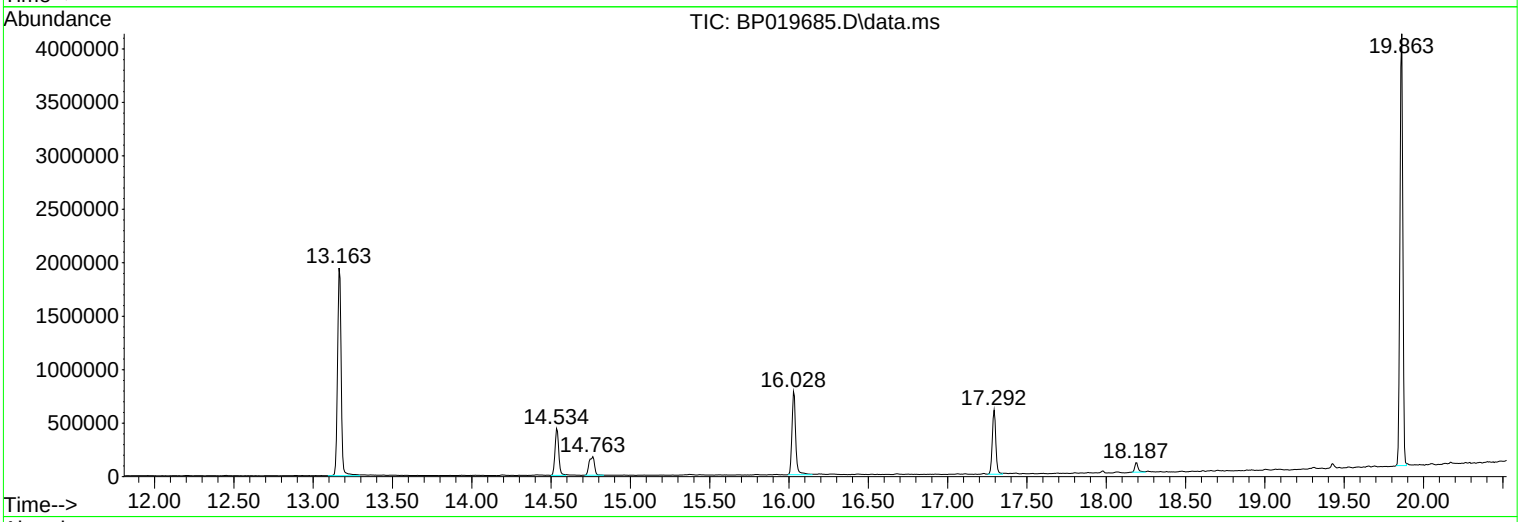
Operator : MA/JU
Sample : P1446-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

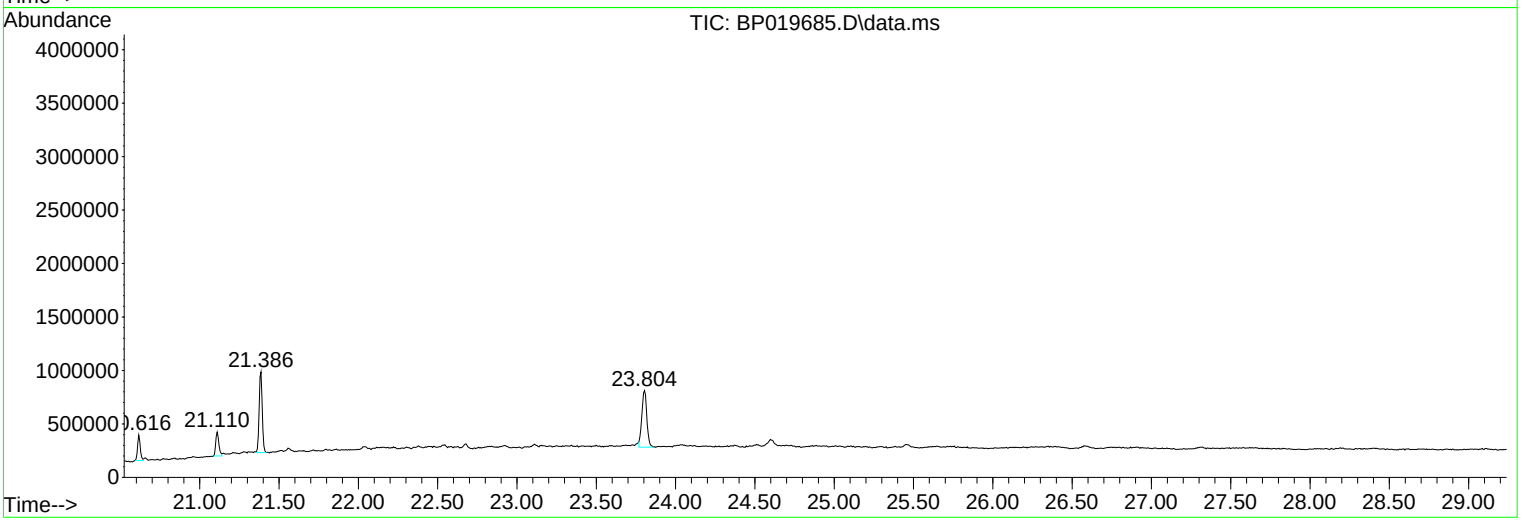
Instrument :
BNA_P
ClientSampleId :
RT3475

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BP019685.D
Acq On : 13 Feb 2024 19:24
Operator : MA/JU
Sample : P1446-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT3475

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

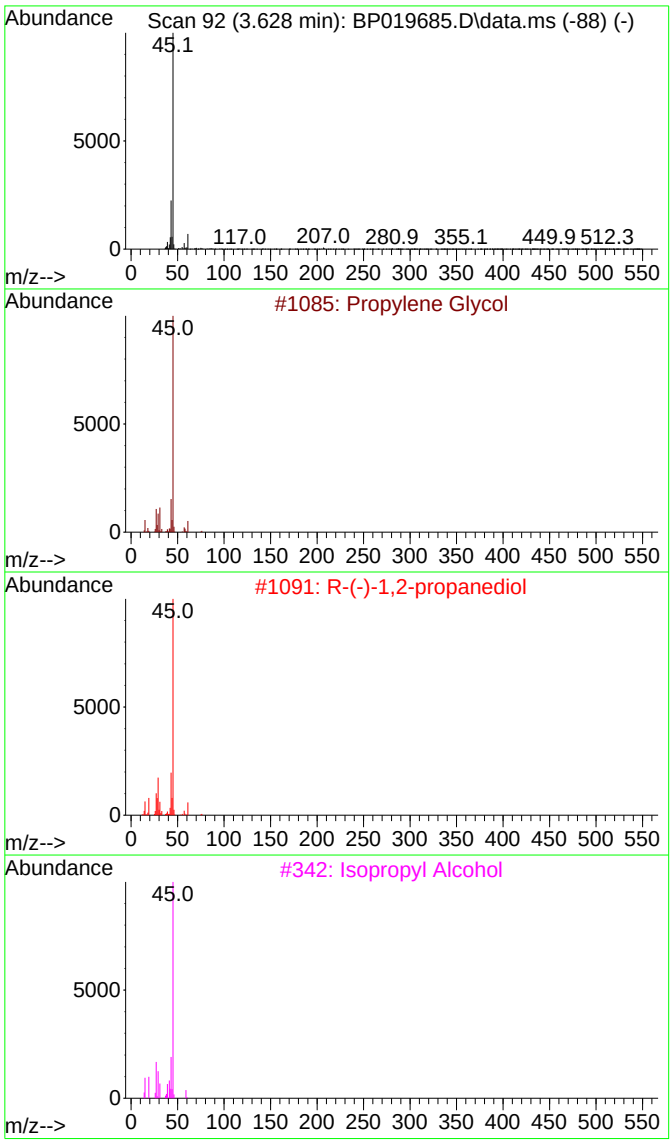
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

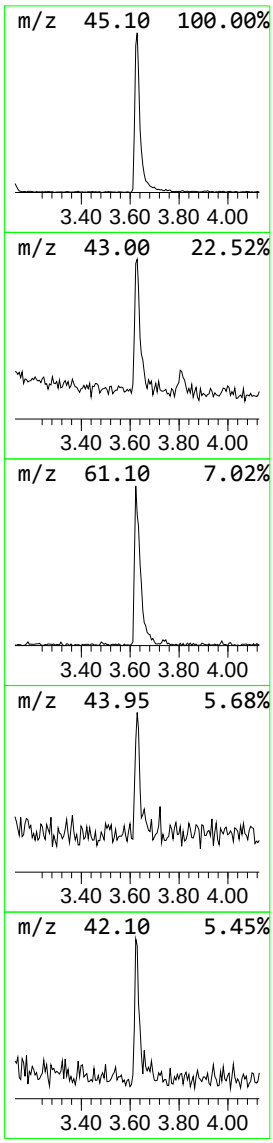
****

Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.628	2.99 ng	59472	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	72
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	56
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	40
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	14
5	2-Hexanol	102	C6H14O	000626-93-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019685.D
Acq On : 13 Feb 2024 19:24
Operator : MA/JU
Sample : P1446-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT3475

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

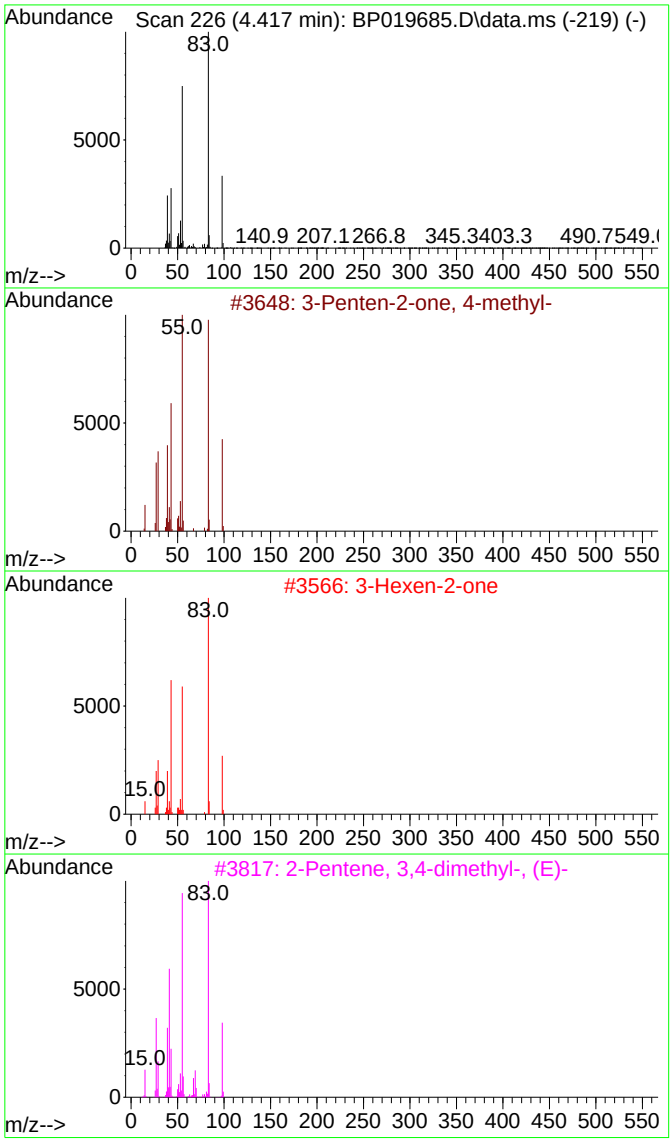
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

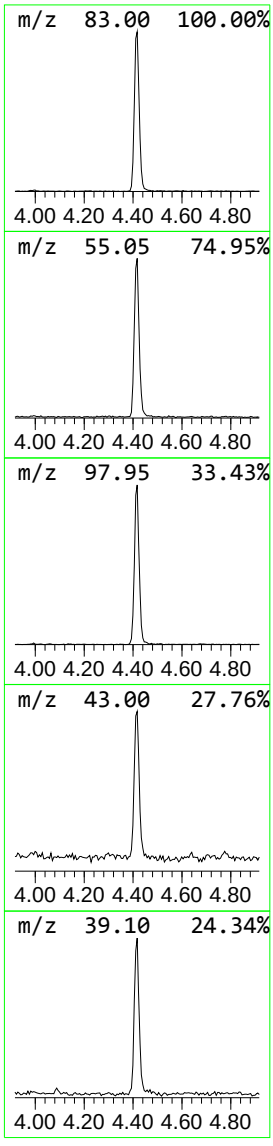
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.417	8.74 ng	173852	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Data File : BP019685.D
Acq On : 13 Feb 2024 19:24
Operator : MA/JU
Sample : P1446-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT3475

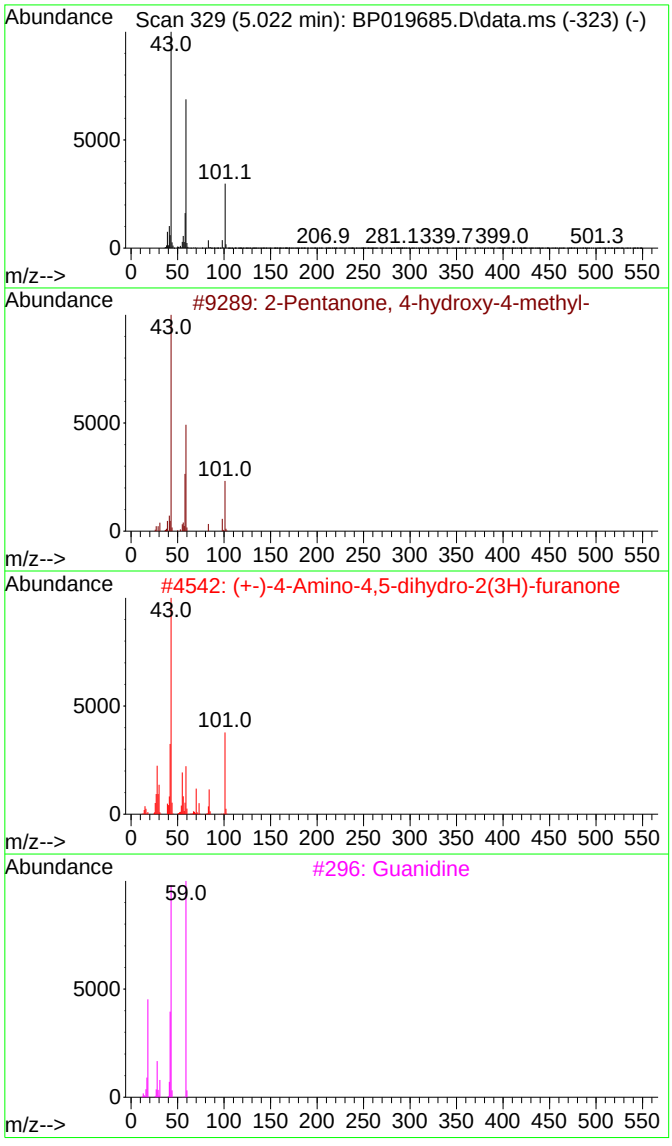
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

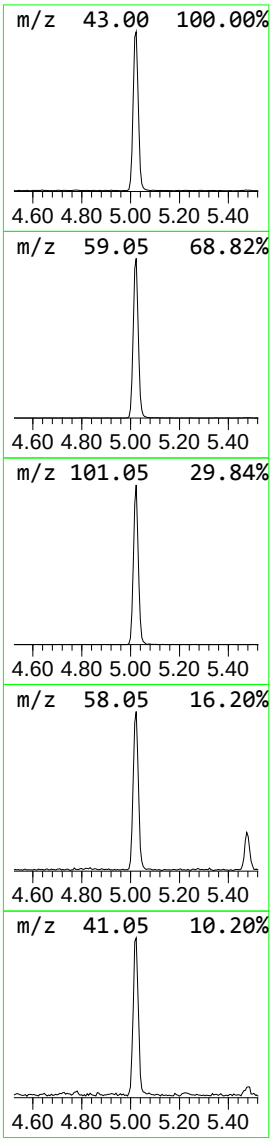
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	29.18 ng	580700	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Data File : BP019685.D
Acq On : 13 Feb 2024 19:24
Operator : MA/JU
Sample : P1446-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT3475

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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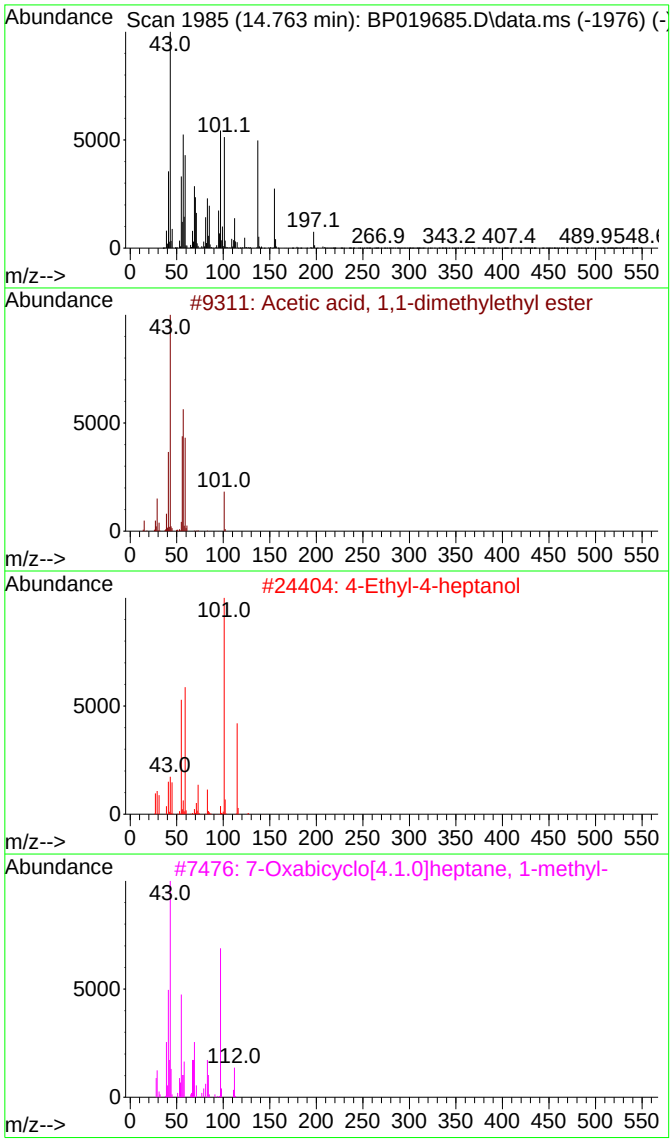
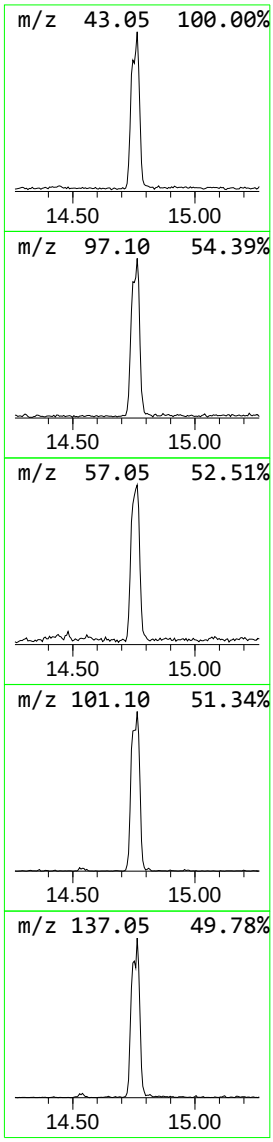
Peak Number 4 unknown14.763 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	11.52 ng	410506	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22
2	4-Ethyl-4-heptanol	144	C9H20O	000597-90-0	22
3	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	11
4	Succinic acid, butyl 4,4-dimethy...	272	C15H28O4	1000381-71-6	10
5	Succinic acid, 4-methylpent-2-yl...	272	C15H28O4	1000349-22-2	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019685.D
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Operator : MA/JU
Sample : P1446-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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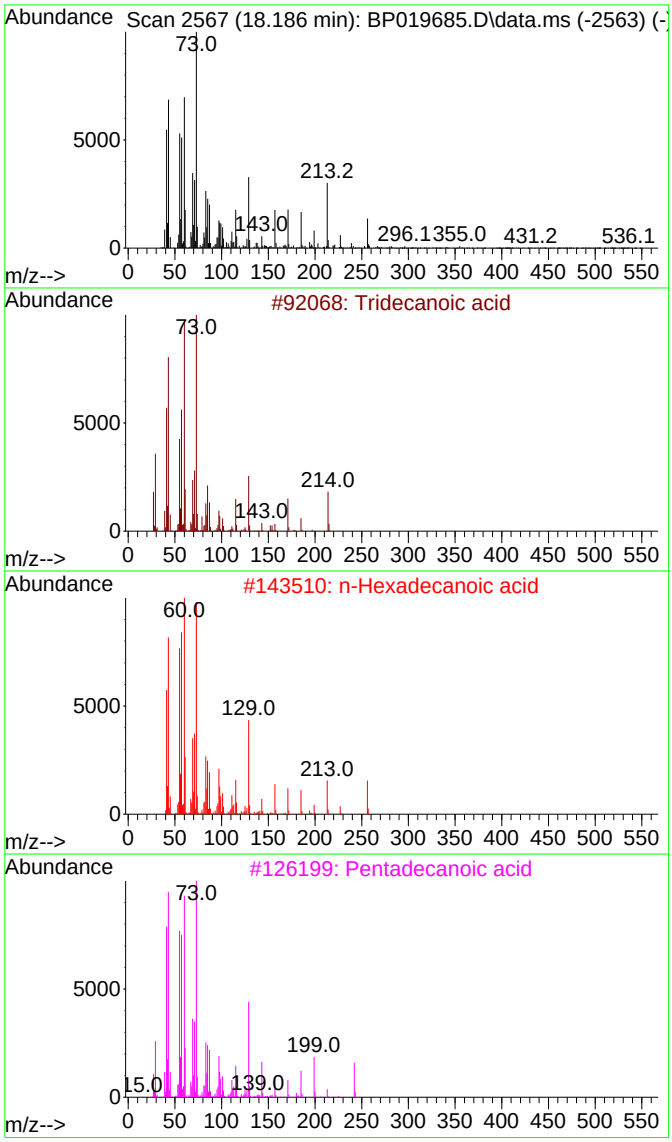
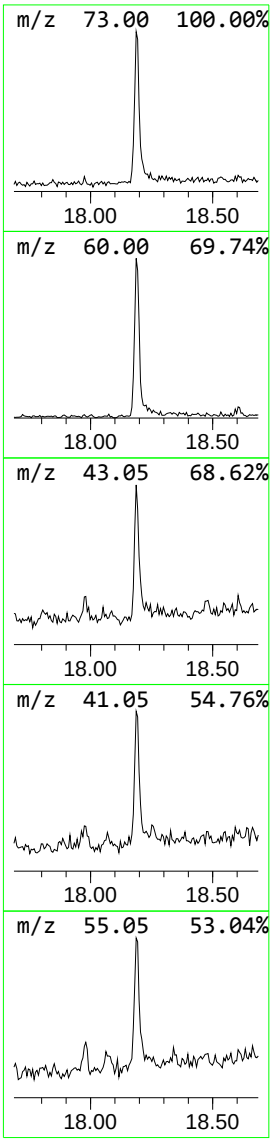
****

Peak Number 5 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	2.92 ng	134677	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





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Sample : P1446-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT3475

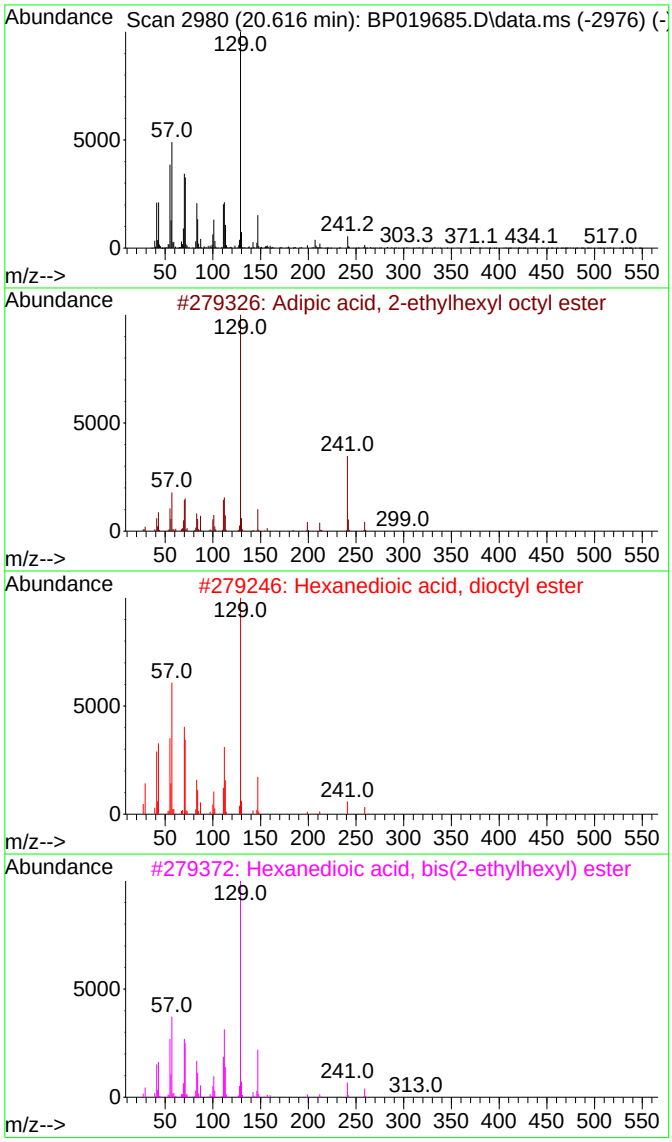
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

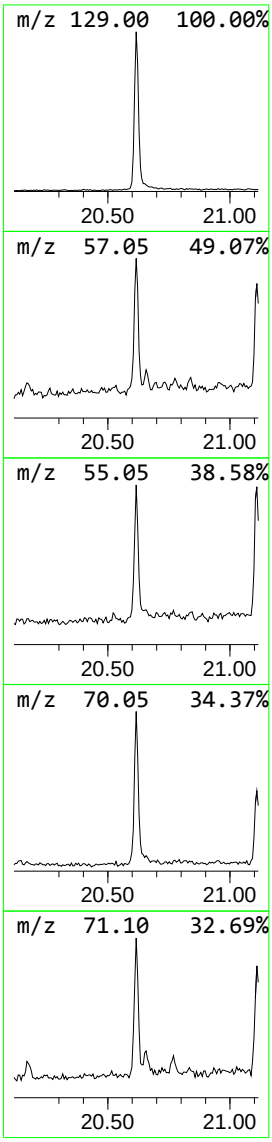
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Adipic acid, 2-ethylhexyl o... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.616	5.55 ng	283712	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
2	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	87
3	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	81
4	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	64
5	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	53





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Instrument :
BNA_P
ClientSampleId :
RT3475

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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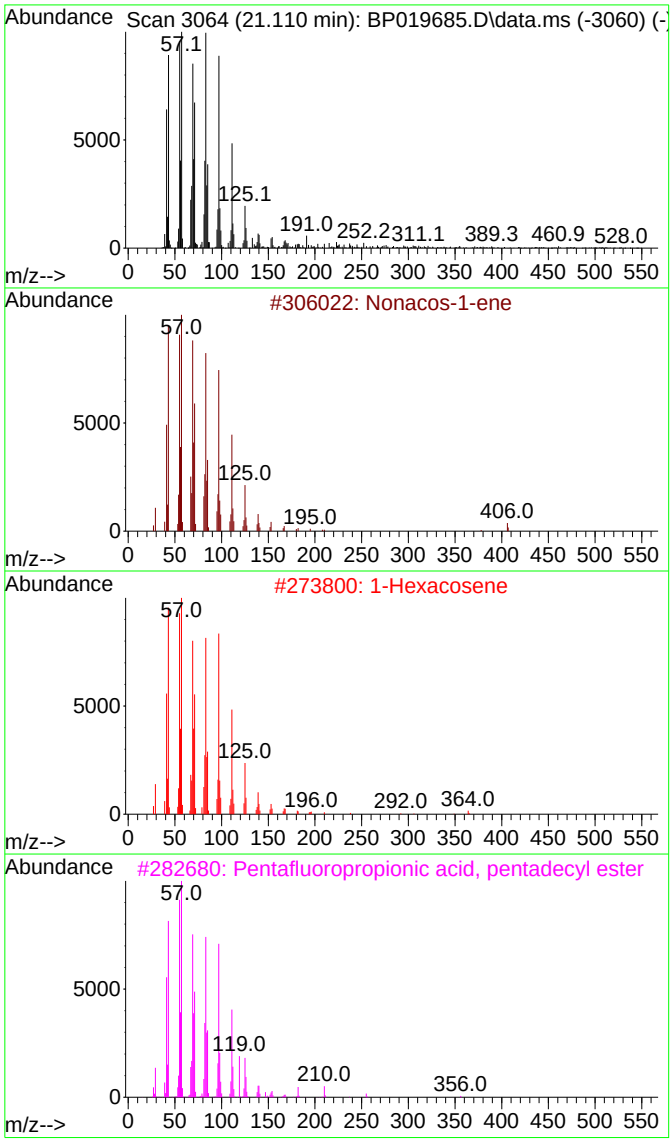
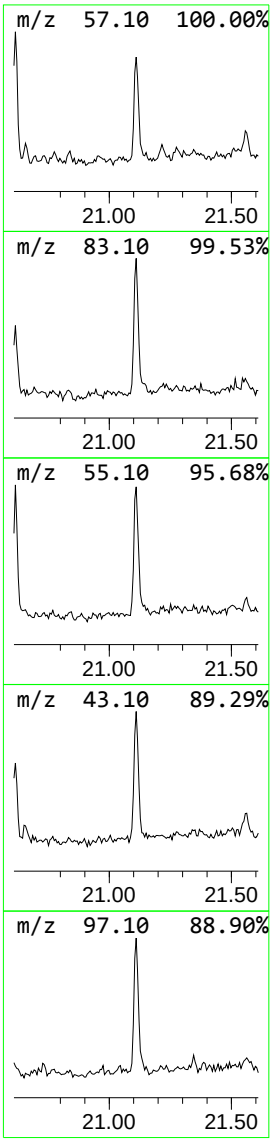
Peak Number 7 Nonacos-1-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.110	5.99 ng	306203	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Heptacos-1-ene	378	C27H54	015306-27-1	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94





Tentatively Identified Compound (LSC) summary

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Data File : BP019685.D
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Misc :
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Instrument :
BNA_P
ClientSampleId :
RT3475

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propylene Glycol	3.628	3.0	ng	59472	1	7.899	397973	20.0
3-Penten-2-one,...	4.417	8.7	ng	173852	1	7.899	397973	20.0
2-Pentanone, 4-...	5.022	29.2	ng	580700	1	7.899	397973	20.0
unknown14.763	14.763	11.5	ng	410506	3	14.534	712491	20.0
Tridecanoic acid	18.186	2.9	ng	134677	4	17.292	921038	20.0
Adipic acid, 2-...	20.616	5.5	ng	283712	5	21.386	1022220	20.0
Nonacos-1-ene	21.110	6.0	ng	306203	5	21.386	1022220	20.0