LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004540.D
Acq On : 13 Jan 2021 16:38
Operator : CG/JU
Sample : M1123-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 355

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-BP011221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004540.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.346	192	197	219	rVB	3554679	5040460	52.03%	10.072%
2	4.946	292	299	312	rBV	3762336	5593516	57.74%	11.177%
3	6.981	637	645	662	rBV	440170	783778	8.09%	1.566%
4	7.811	778	786	793	rBV	658573	1068835	11.03%	2.136%
5	8.969	975	983	1006	rBV	1298309	2212936	22.85%	4.422%
6	10.605	1252	1261	1269	rBV	831180	1447903	14.95%	2.893%
7	13.075	1673	1681	1693	rBV	3990742	6171061	63.71%	12.331%
8	13.881	1813	1818	1820	rBV	99812	137143	1.42%	0.274%
9	13.910	1820	1823	1827	rVB	149747	205409	2.12%	0.410%
10	14.198	1866	1872	1878	rBV4	65162	154514	1.60%	0.309%
11	14.293	1884	1888	1895	rVB3	189152	286087	2.95%	0.572%
12	14.363	1895	1900	1906	rBV2	105629	172560	1.78%	0.345%
13	14.463	1907	1917	1925	rVV	1342931	2199003	22.70%	4.394%
14	14.987	2003	2006	2013	rBV4	105412	181571	1.87%	0.363%
15	15.181	2036	2039	2045	rBV5	58633	106630	1.10%	0.213%
16	15.257	2047	2052	2056	rBV2	196526	289146	2.98%	0.578%
17	15.734	2130	2133	2139	rVB	134103	195435	2.02%	0.391%
18	15.940	2165	2168	2172	rBV2	111433	173654	1.79%	0.347%
19	16.210	2207	2214	2219	rBV2	392247	836337	8.63%	1.671%
20	17.039	2352	2355	2366	rVB	343543	598623	6.18%	1.196%
21	17.222	2381	2386	2391	rBV	1721091	2645123	27.31%	5.285%
22	19.239	2726	2729	2735	rVB	626283	838944	8.66%	1.676%
23	19.786	2818	2822	2832	rVB	7326923	9686726	100.00%	19.356%
24	21.022	3029	3032	3041	rVB3	945727	1664609	17.18%	3.326%
25	21.222	3064	3066	3072	rVB	482733	527692	5.45%	1.054%
26	21.316	3077	3082	3087	rBV	2413116	3491379	36.04%	6.976%
27	23.674	3476	3483	3490	rBV2	1706604	3336549	34.44%	6.667%

Sum of corrected areas: 50045623

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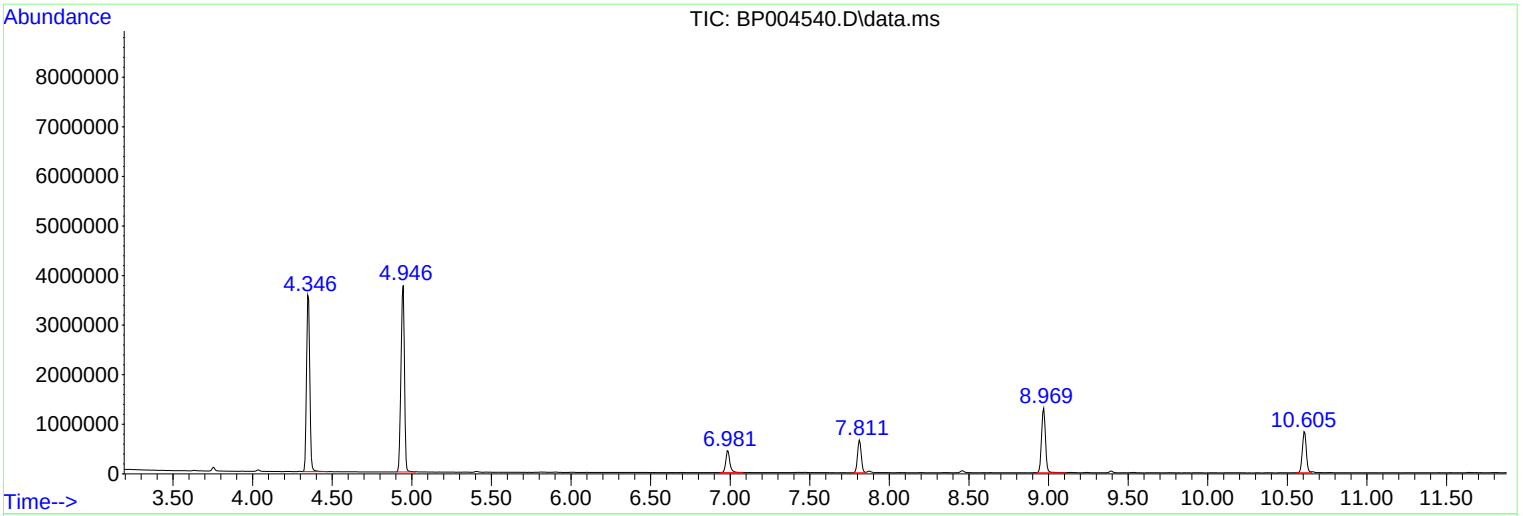
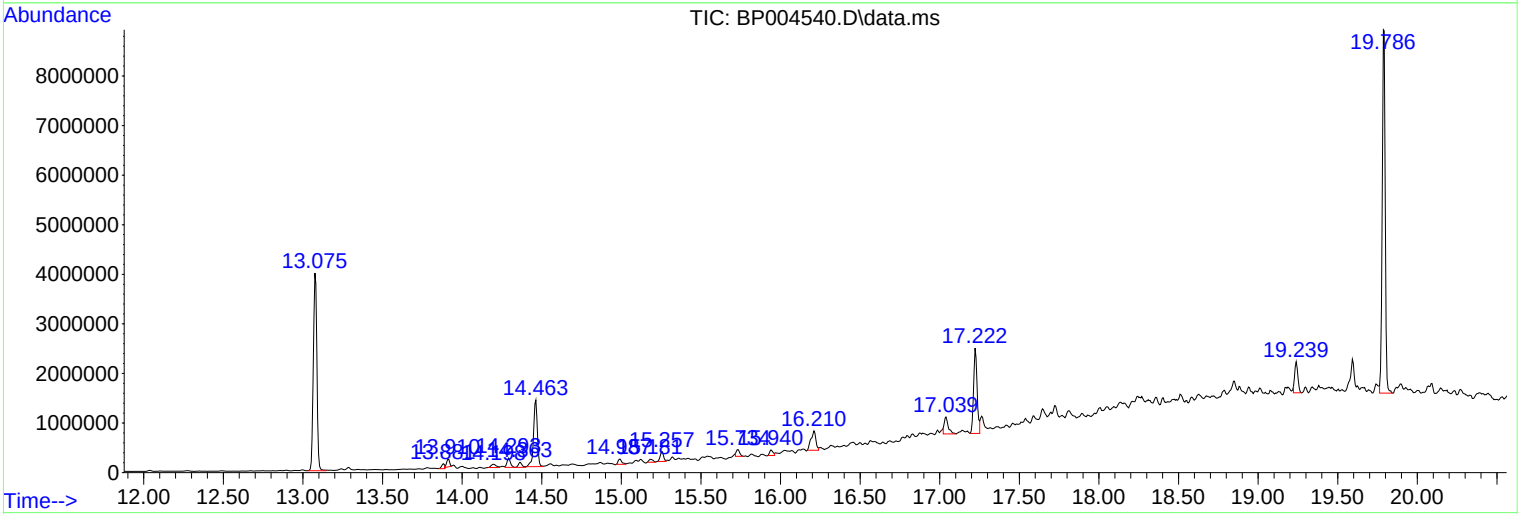
Misc :
ALS Vial : 13 Sample Multiplier: 1

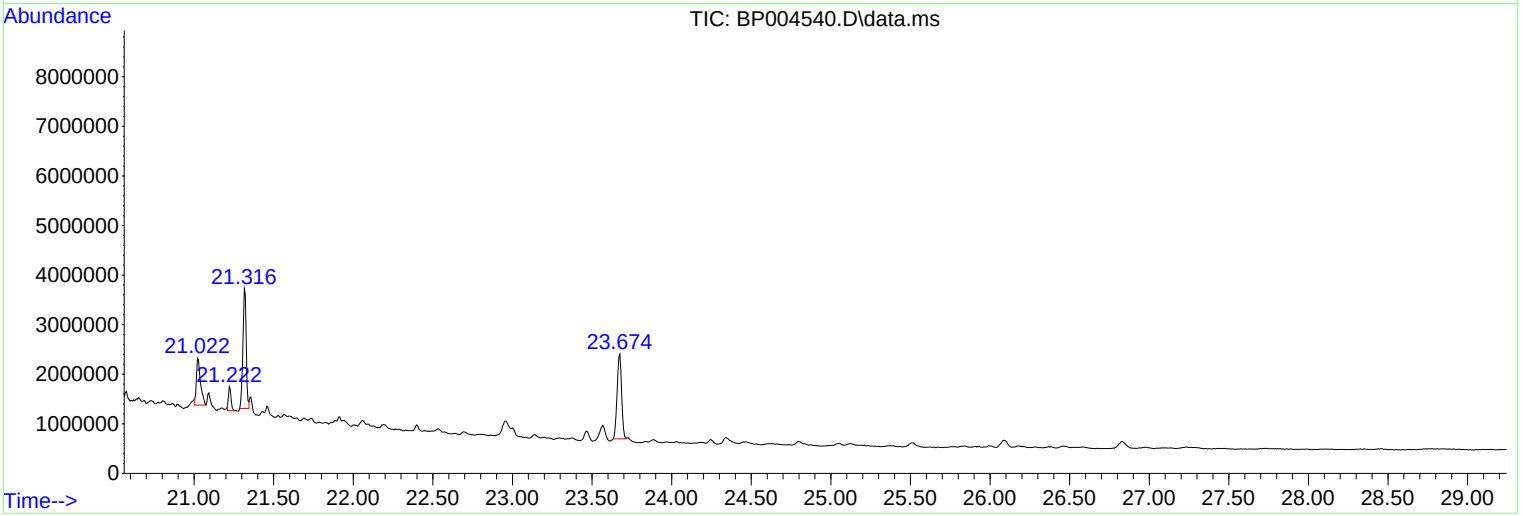
Instrument :
BNA_P
ClientSampleId :
355

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.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\BP011321\
Data File : BP004540.D
Acq On : 13 Jan 2021 16:38
Operator : CG/JU
Sample : M1123-01
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

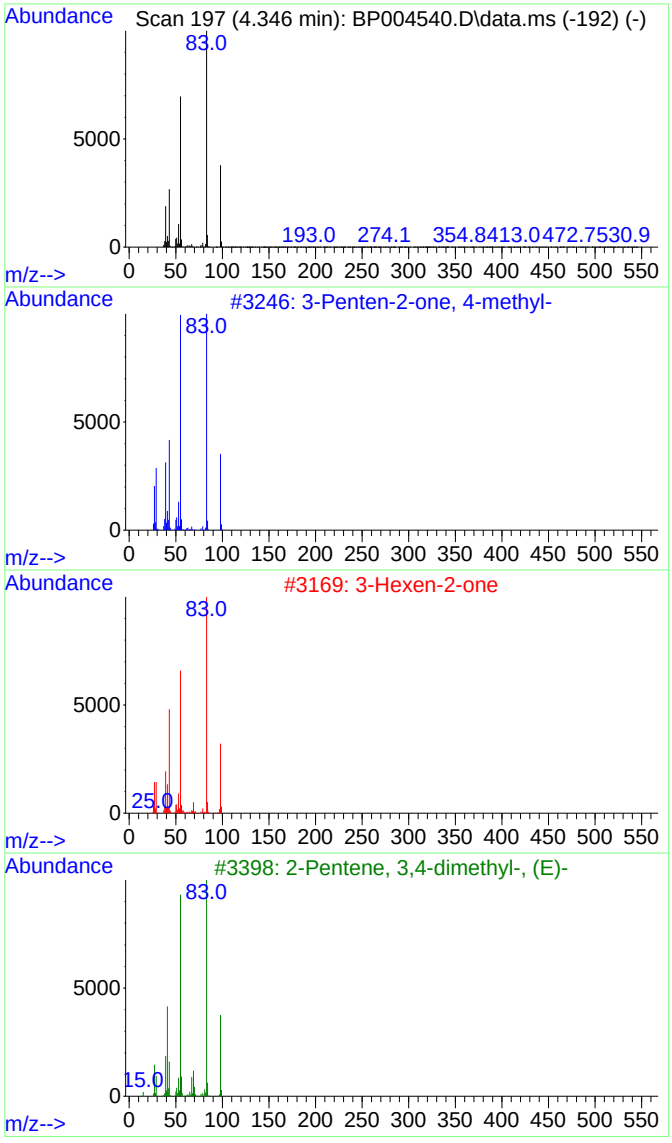
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

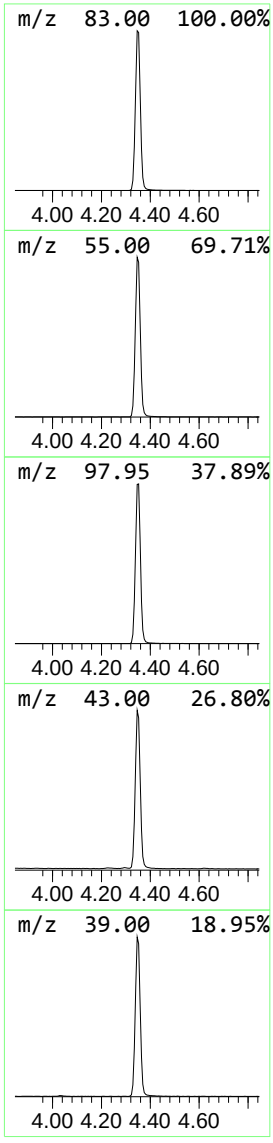
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.346	94.32 ng	5040460	1,4-Dichlorobenzene-d4	7.811

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	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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Data File : BP004540.D
Acq On : 13 Jan 2021 16:38
Operator : CG/JU
Sample : M1123-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
355

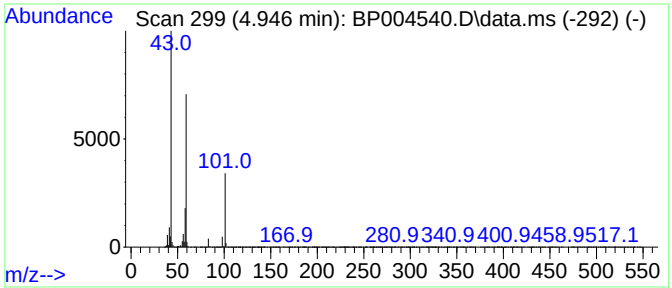
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

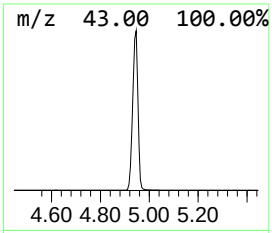
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

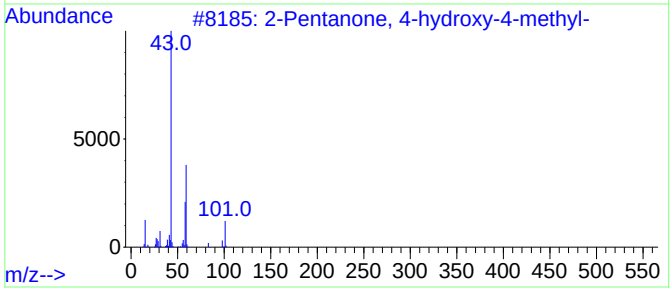
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

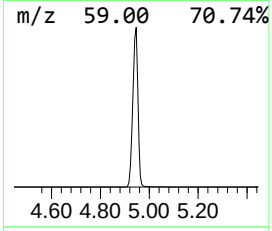
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	104.67 ng	5593520	1,4-Dichlorobenzene-d4	7.811

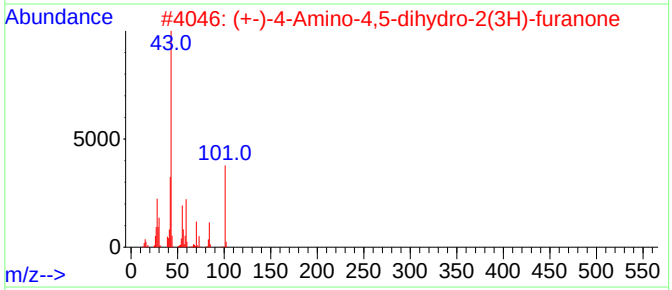
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9

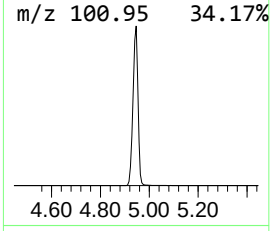


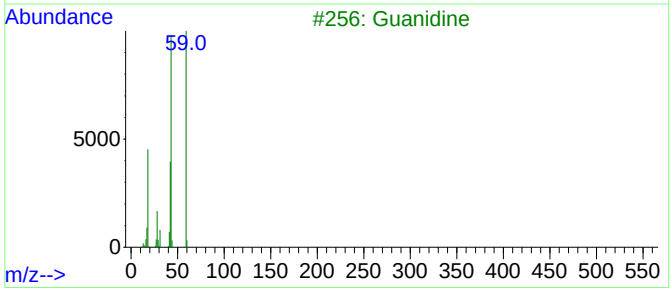


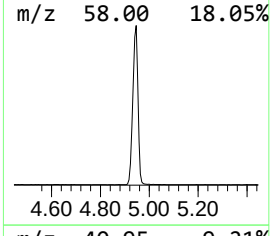


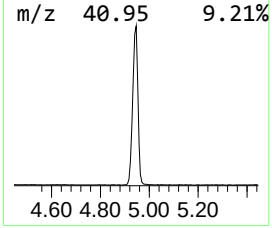












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004540.D
Acq On : 13 Jan 2021 16:38
Operator : CG/JU
Sample : M1123-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
355

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

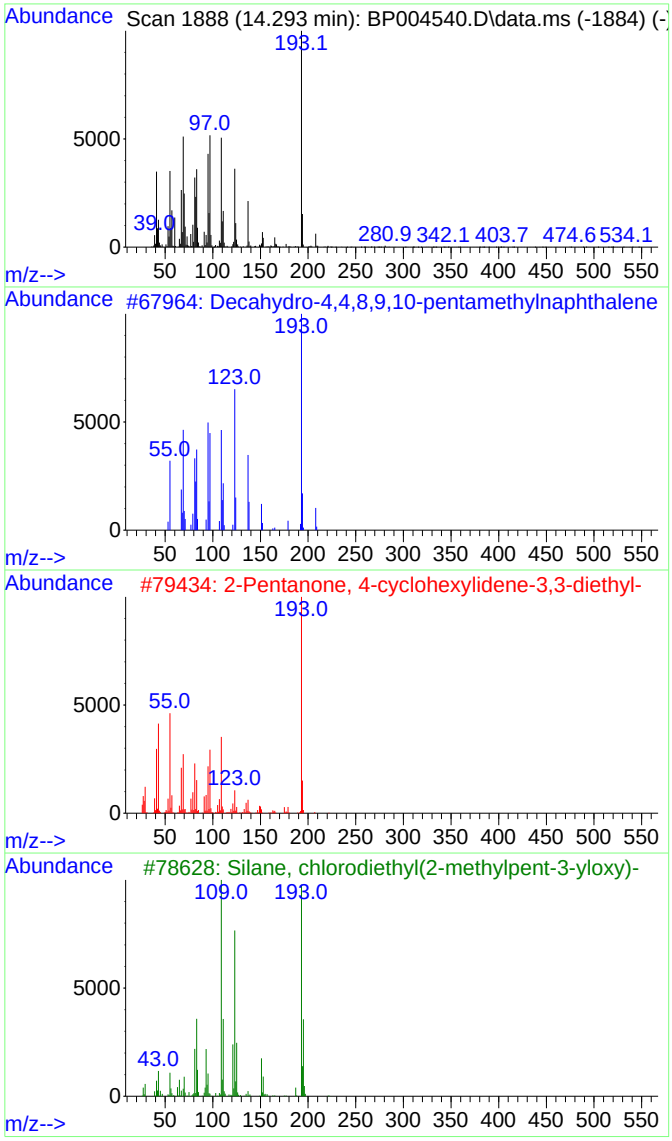
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

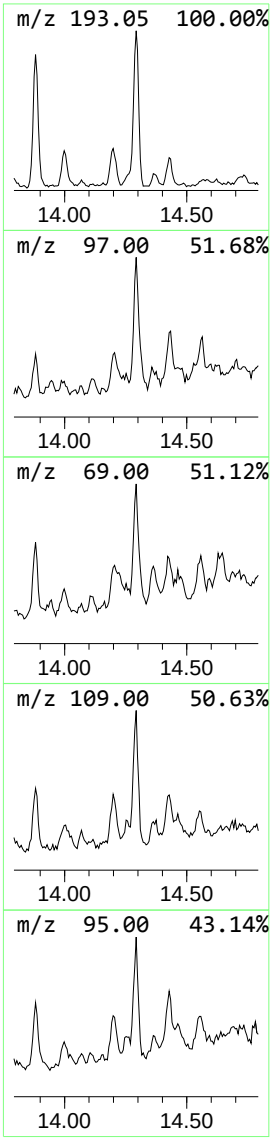
****

Peak Number 3 unknown14.29 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.293	2.60 ng	286087	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	49
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
3	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	38
4	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
5	1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1000298-97-4	37





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Instrument :
BNA_P
ClientSampleId :
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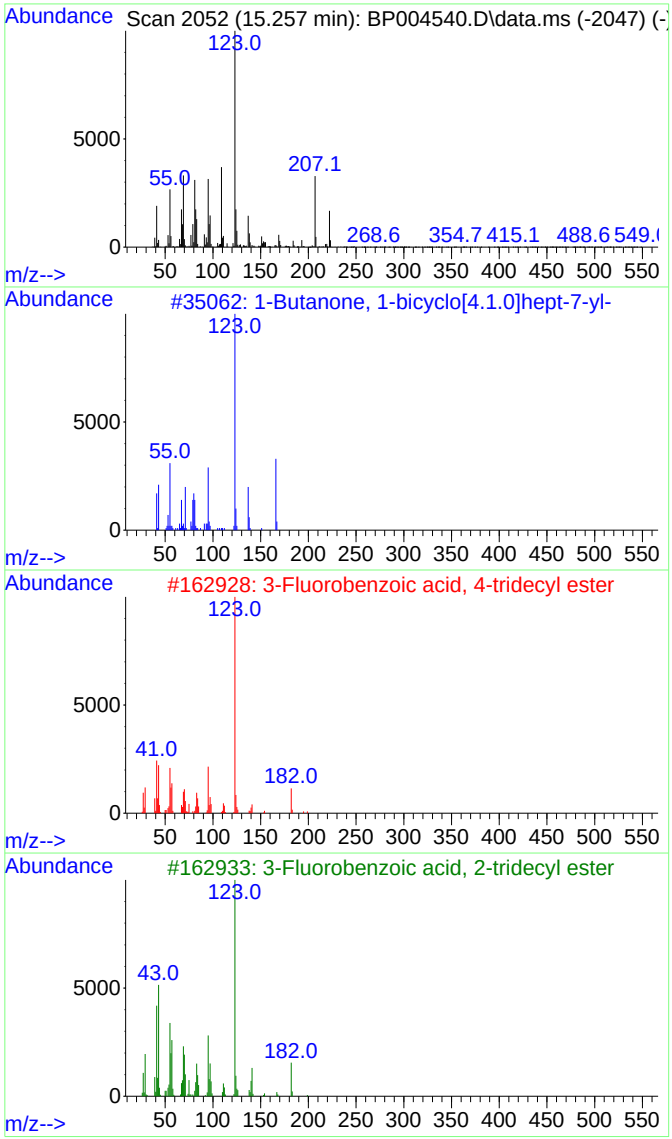
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

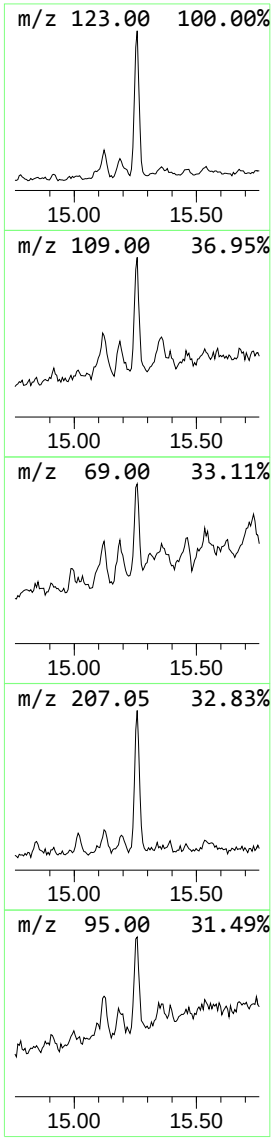
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Butanone, 1-bicyclo[4.1.0... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.257	2.63 ng	289146	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	50
2	3-Fluorobenzoic acid, 4-tridecyl...	322	C20H31FO2	1000280-60-4	50
3	3-Fluorobenzoic acid, 2-tridecyl...	322	C20H31FO2	1000280-60-2	50
4	4-Fluorobenzoic acid, 3-tetradec...	336	C21H33FO2	1000280-68-1	50
5	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	50





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Instrument : BNA_P
ClientSampleId : 355

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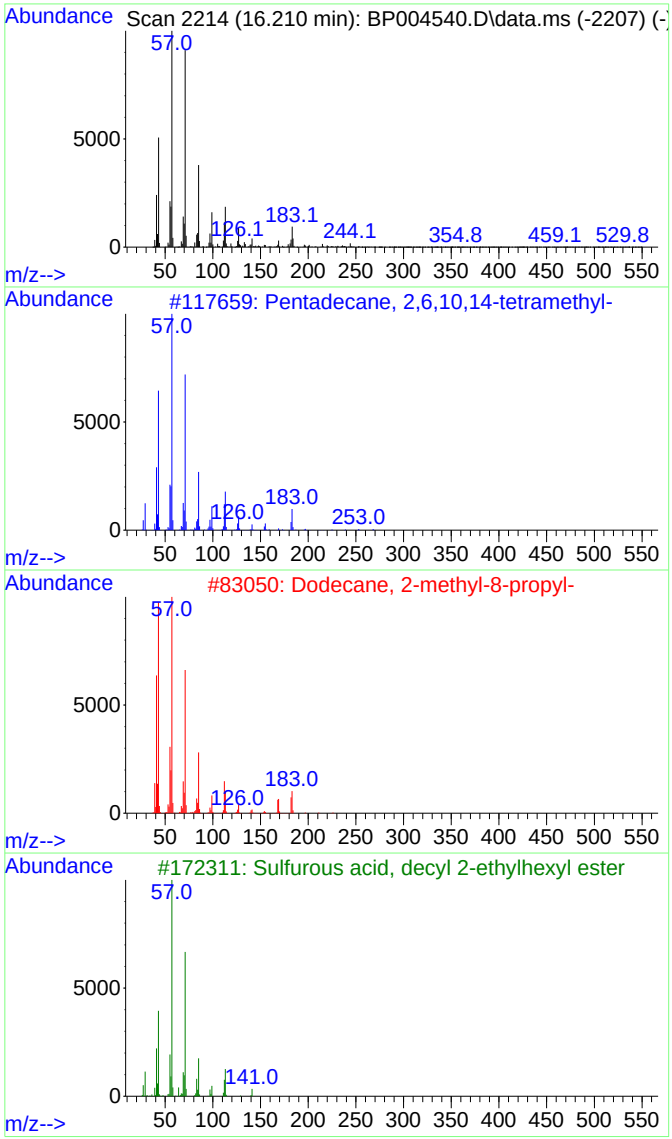
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

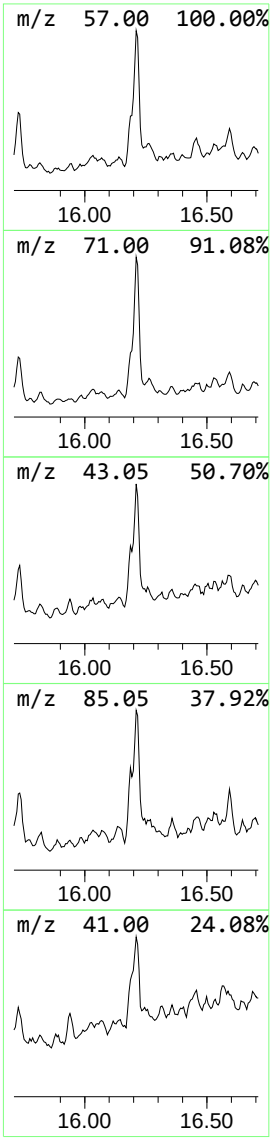
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecane, 2,6,10,14-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.210	6.32 ng	836337	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	91
2	Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	90
3	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	74
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	72
5	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	72





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Instrument : BNA_P
ClientSampleId : 355

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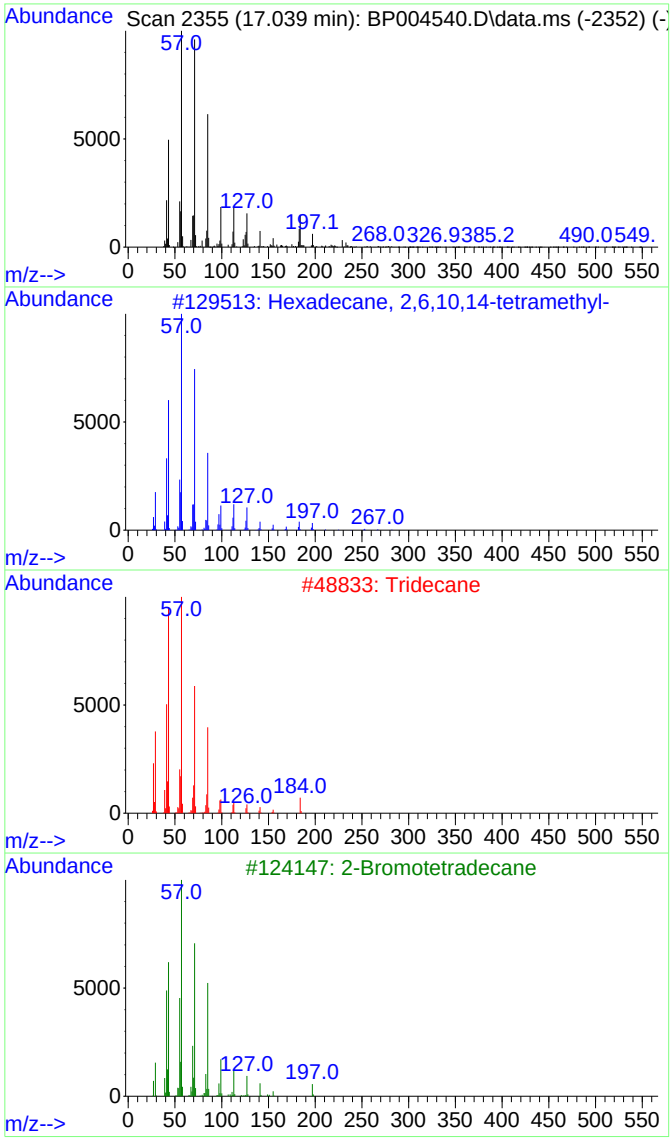
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

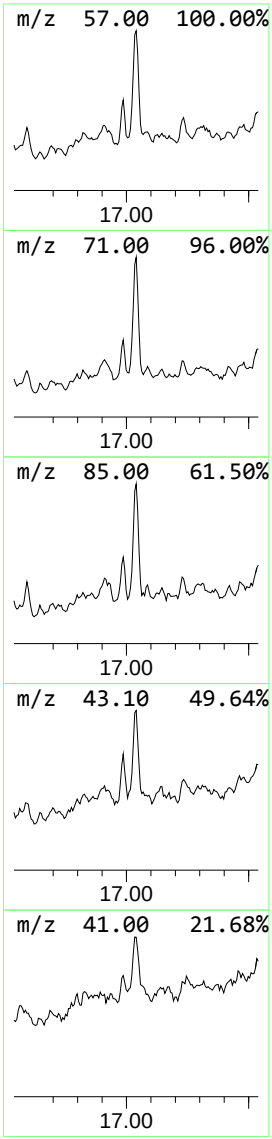
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.040	4.53 ng	598623	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	93
2	Tridecane	184	C13H28	000629-50-5	87
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Heneicosane	296	C21H44	000629-94-7	80





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Instrument : BNA_P
ClientSampleId : 355

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

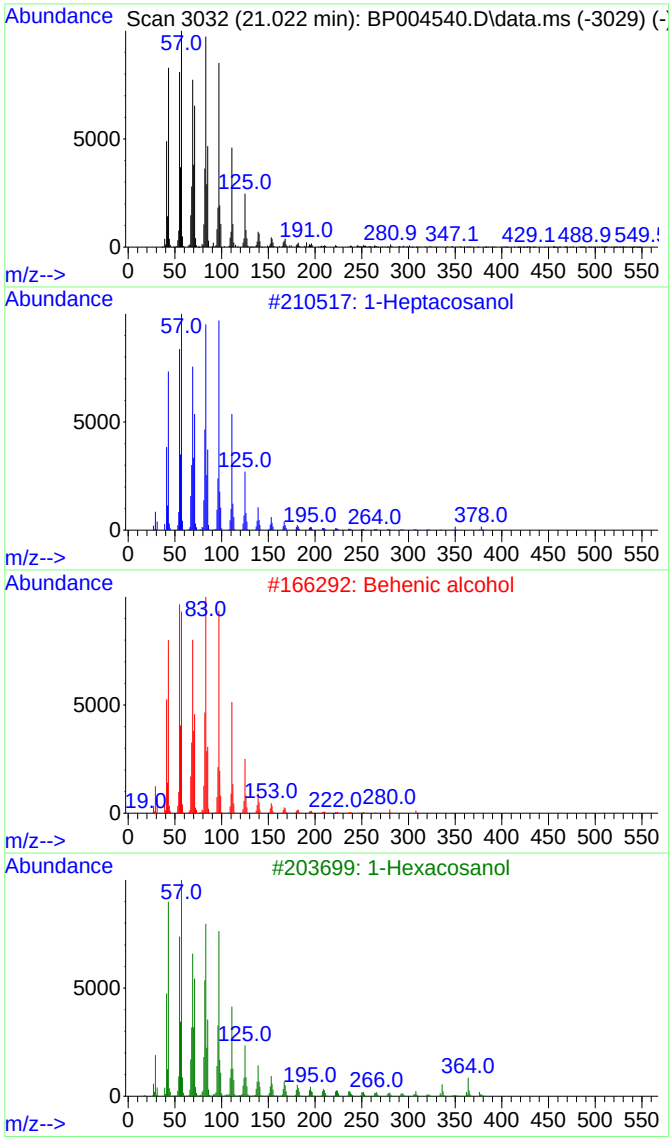
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

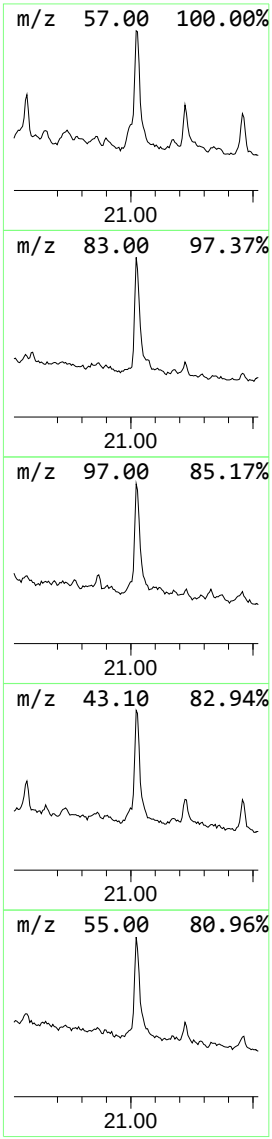
****

Peak Number 7 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	9.54 ng	1664610	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Hexacosanol	382	C26H54O	000506-52-5	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004540.D
Acq On : 13 Jan 2021 16:38
Operator : CG/JU
Sample : M1123-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 355

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.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
3-Penten-2-one,...	4.346	94.3	ng	5040460	1	7.811	1068840	20.0
2-Pentanone, 4-...	4.946	104.7	ng	5593520	1	7.811	1068840	20.0
unknown14.29	14.293	2.6	ng	286087	3	14.463	2199000	20.0
1-Butanone, 1-b...	15.257	2.6	ng	289146	3	14.463	2199000	20.0
Pentadecane, 2,...	16.210	6.3	ng	836337	4	17.222	2645120	20.0
Hexadecane, 2,6...	17.040	4.5	ng	598623	4	17.222	2645120	20.0
1-Heptacosanol	21.022	9.5	ng	1664610	5	21.316	3491380	20.0