

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112420\
 Data File : BP004080.D
 Acq On : 24 Nov 2020 17:35
 Operator : CG/JU
 Sample : L4597-01 2X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BU-03-112320

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-BP110320.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004080.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.917	3	5	25	rVB	3345510	4566576	56.19%	11.659%
2	3.075	26	32	42	rVV	62141	136370	1.68%	0.348%
3	3.164	43	47	60	rVB	109609	171839	2.11%	0.439%
4	5.799	488	495	509	rBV	732685	1175943	14.47%	3.002%
5	7.452	765	776	788	rBV	728218	1271935	15.65%	3.247%
6	8.263	907	914	922	rBV	483653	771679	9.50%	1.970%
7	9.428	1104	1112	1122	rBV	460090	777372	9.57%	1.985%
8	11.098	1384	1396	1413	rBV	619912	1078585	13.27%	2.754%
9	13.510	1799	1806	1819	rBV	1028691	1515491	18.65%	3.869%
10	14.892	2035	2041	2049	rVB	920296	1333177	16.41%	3.404%
11	16.375	2288	2293	2305	rBV	745765	1088633	13.40%	2.779%
12	17.628	2500	2506	2511	rBV	1027595	1506530	18.54%	3.846%
13	18.239	2605	2610	2619	rVB	1518006	1824331	22.45%	4.658%
14	18.469	2645	2649	2653	rBV2	56833	85556	1.05%	0.218%
15	19.327	2789	2795	2797	rBV	6697253	8126305	100.00%	20.747%
16	19.357	2797	2800	2809	rVB2	5775121	7131533	87.76%	18.207%
17	19.475	2816	2820	2825	rBV	1102152	1214806	14.95%	3.101%
18	20.122	2925	2930	2936	rBV	1531700	1863052	22.93%	4.757%
19	20.522	2995	2998	3001	rBV	123680	131221	1.61%	0.335%
20	21.116	3095	3099	3103	rVB3	90821	162050	1.99%	0.414%
21	21.316	3130	3133	3143	rVB2	107547	189704	2.33%	0.484%
22	21.433	3151	3153	3159	rVB2	112850	126100	1.55%	0.322%
23	21.663	3187	3192	3197	rVB	1088727	1445807	17.79%	3.691%
24	24.139	3606	3613	3620	rVB	723241	1473824	18.14%	3.763%

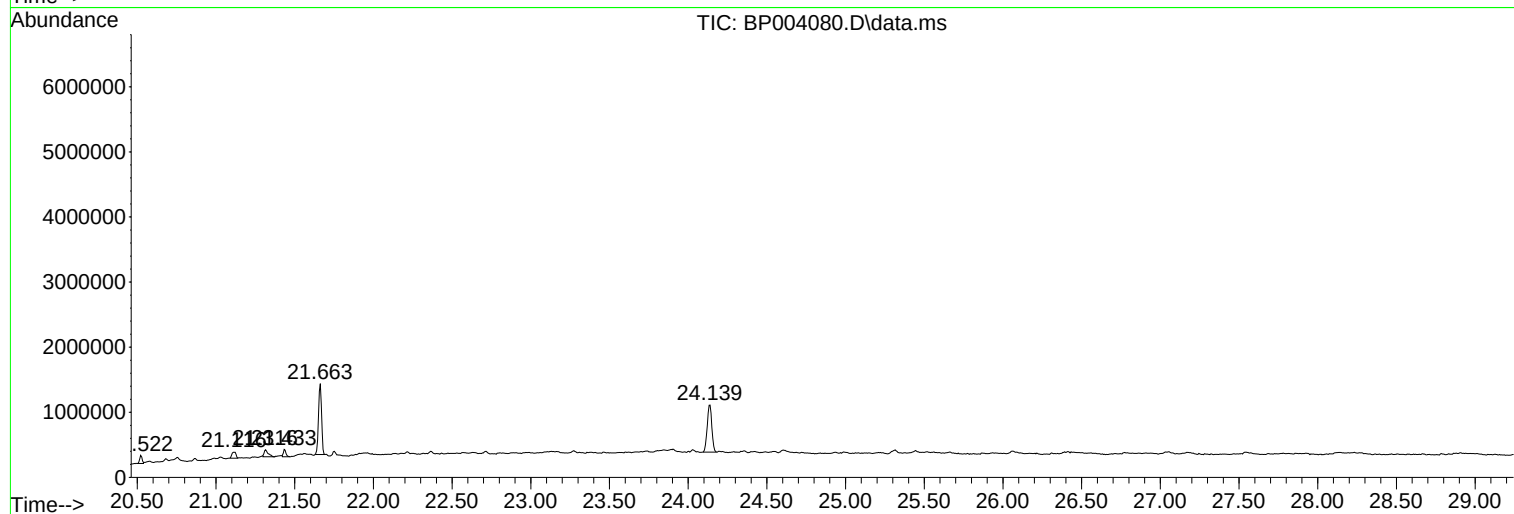
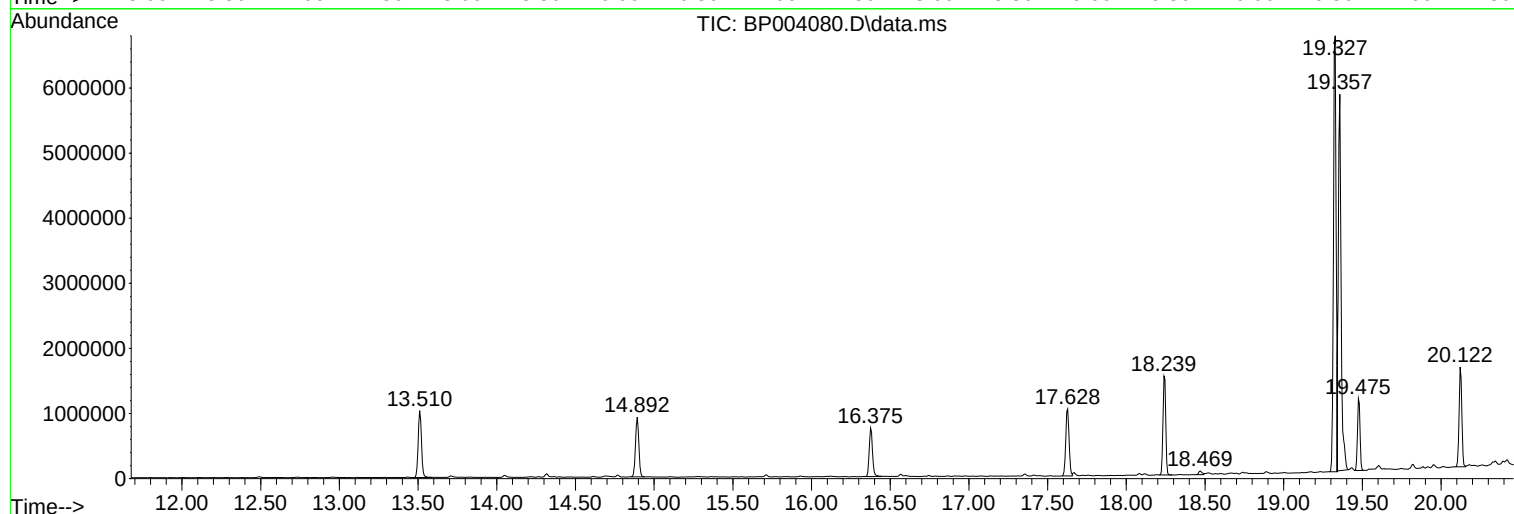
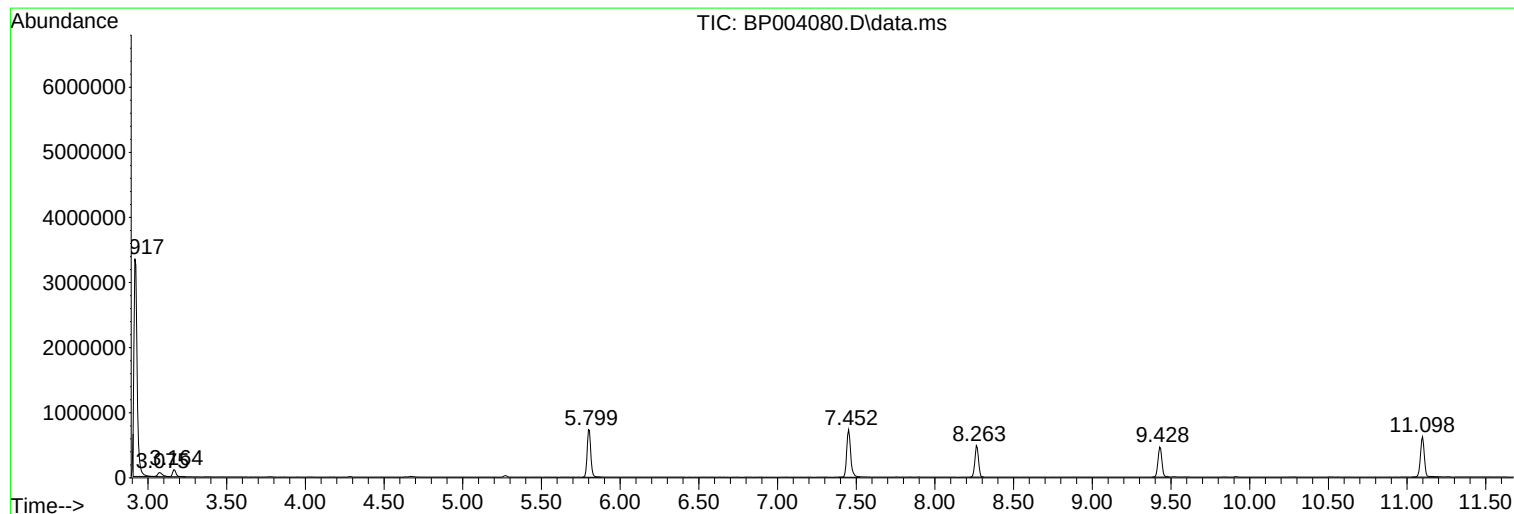
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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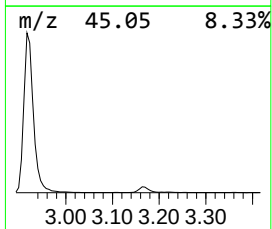
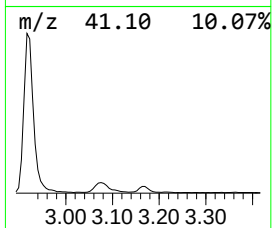
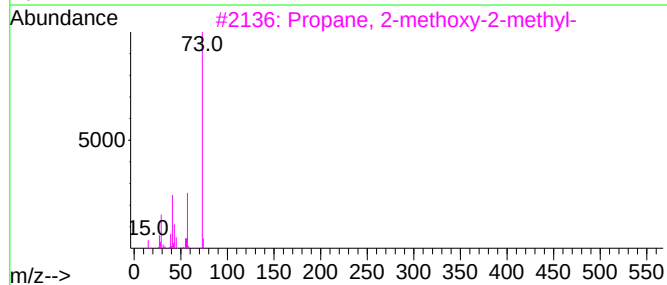
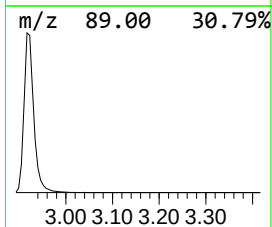
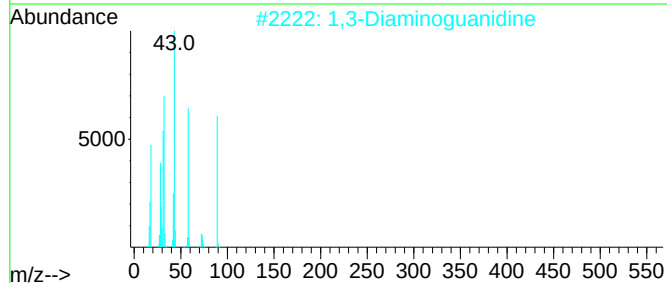
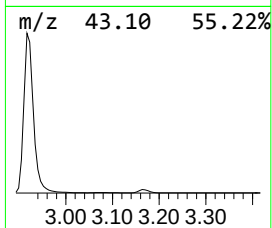
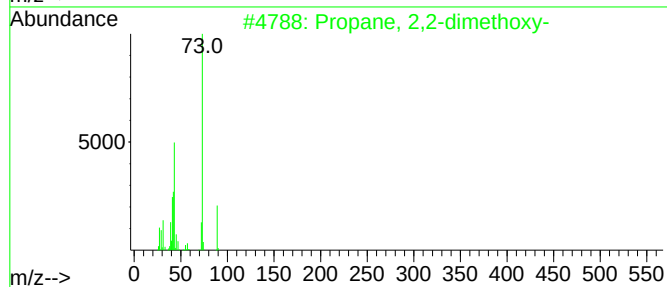
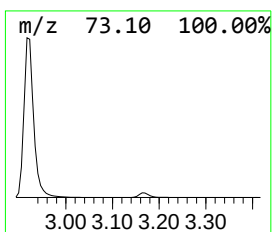
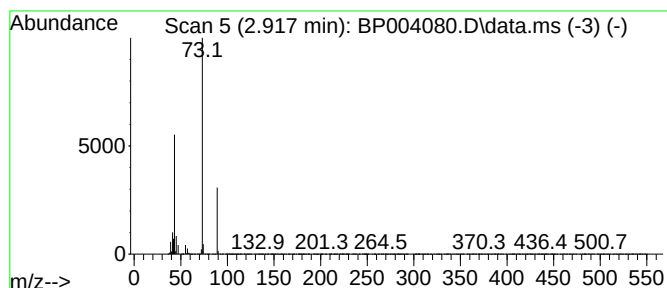
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.917	118.35 ng	4566580	1,4-Dichlorobenzene-d4	8.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4			1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrC13O2	1000115-31-4	9



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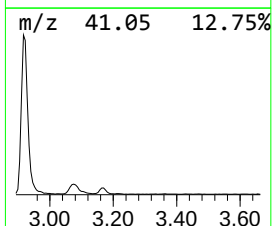
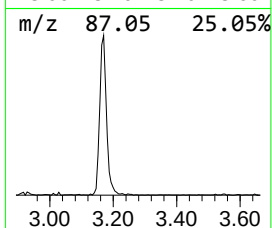
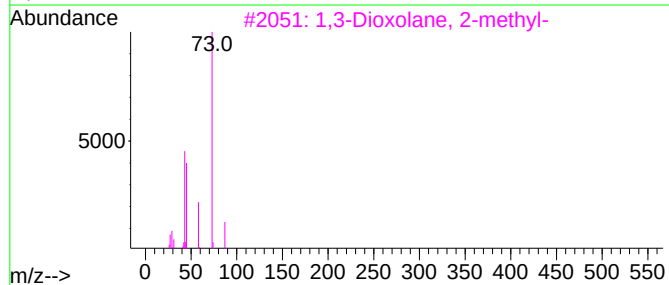
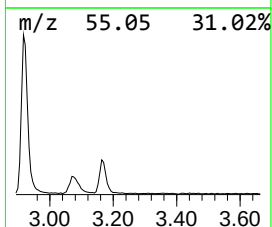
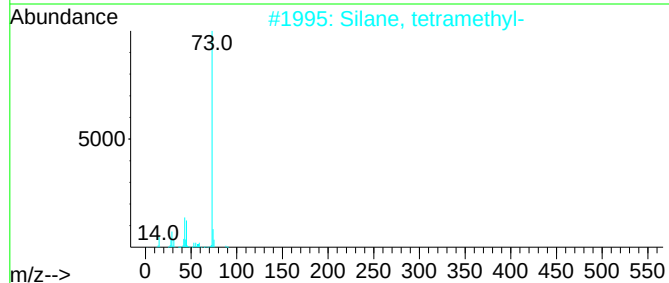
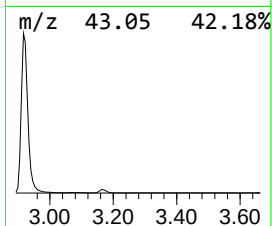
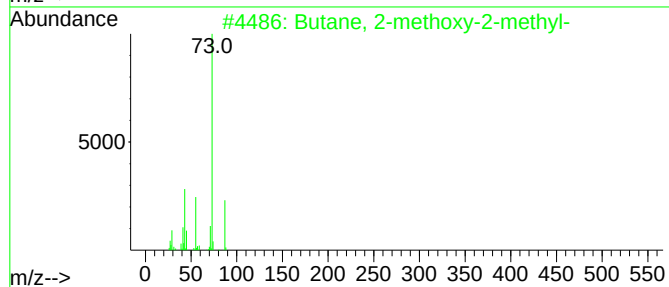
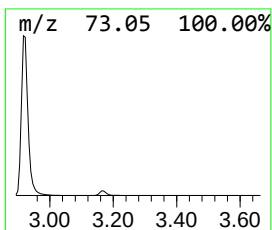
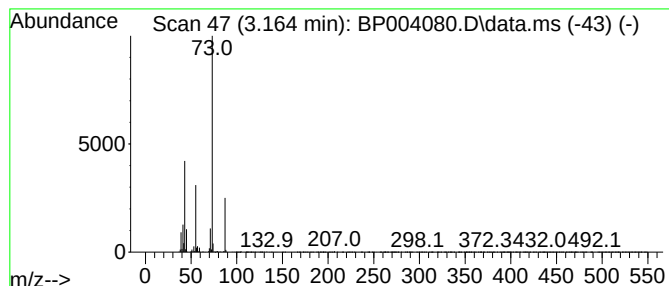
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.164	4.45 ng	171839	1,4-Dichlorobenzene-d4	8.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23



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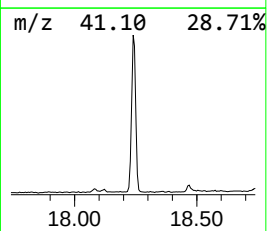
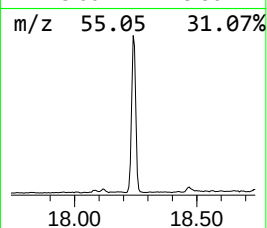
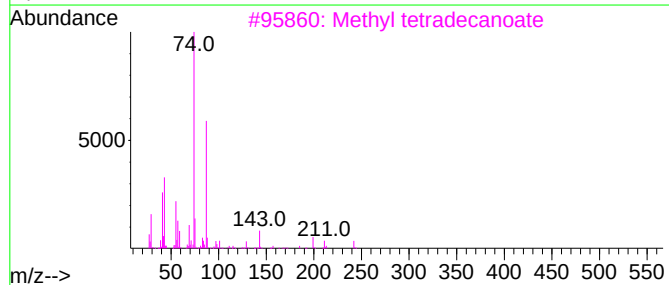
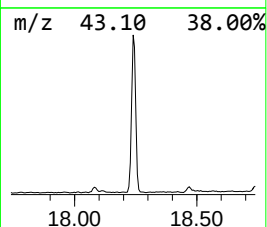
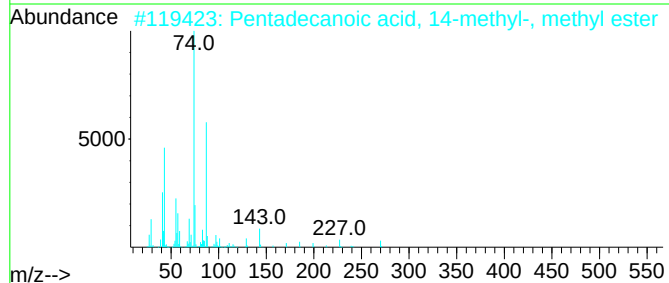
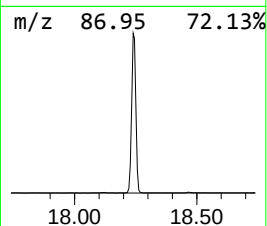
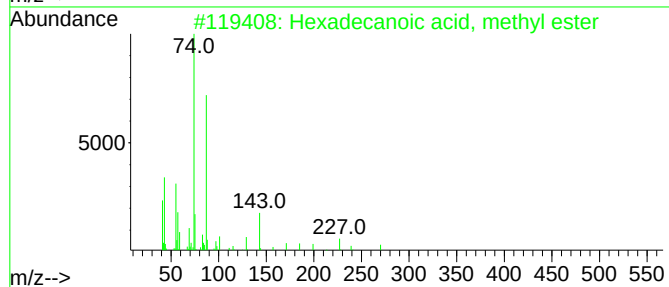
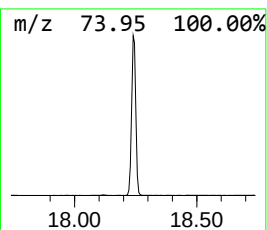
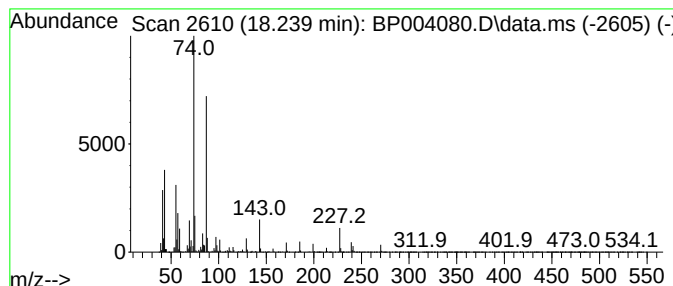
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	24.22 ng	1824330	Phenanthrene-d10	17.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83



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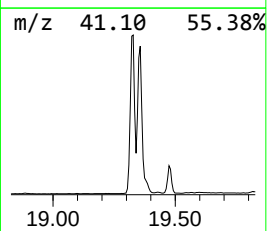
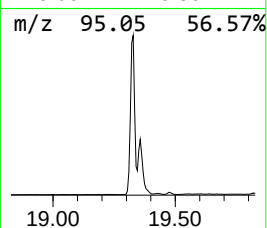
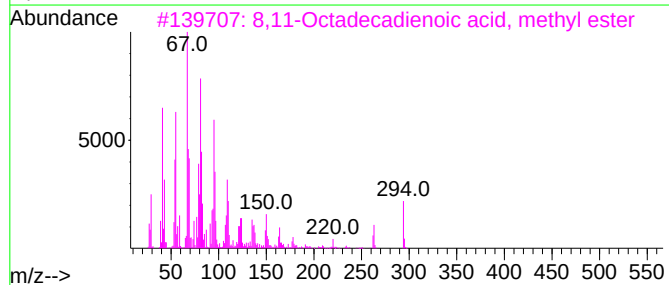
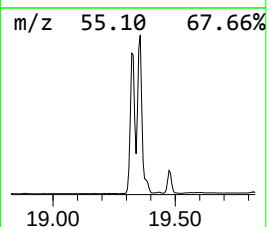
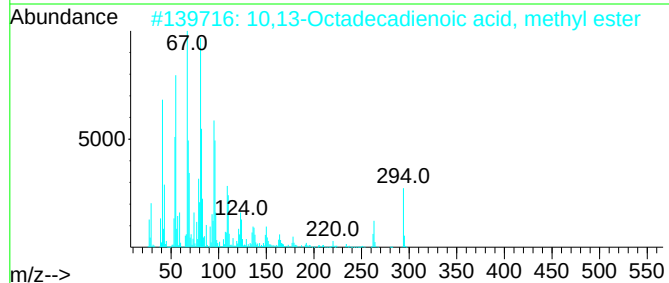
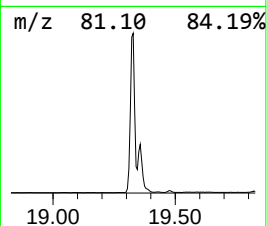
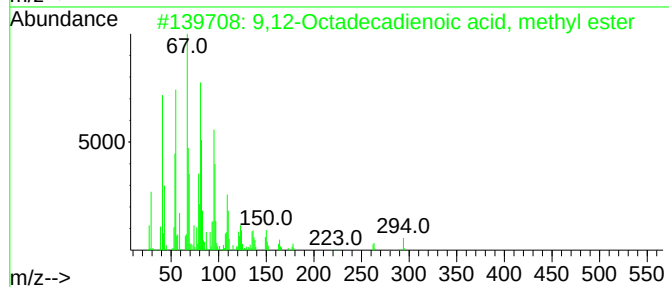
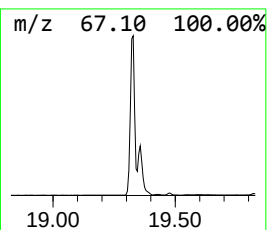
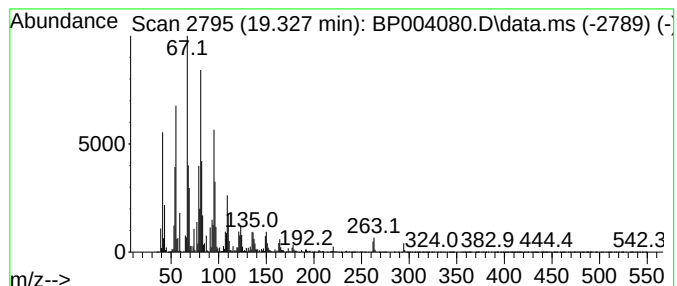
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Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.328	107.88 ng	8126310	Phenanthrene-d10	17.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2			10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3			8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
4			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99



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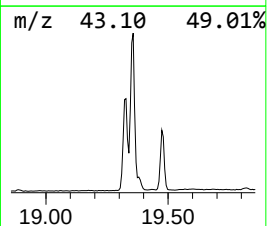
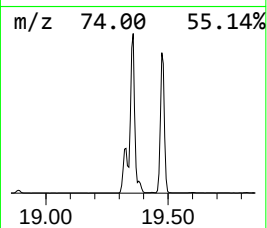
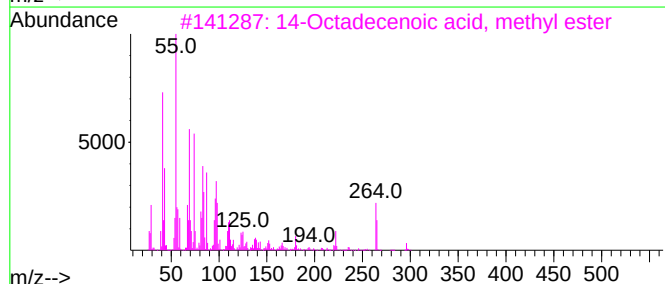
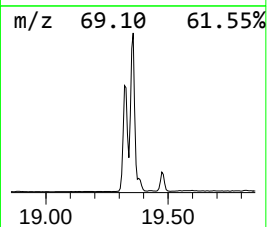
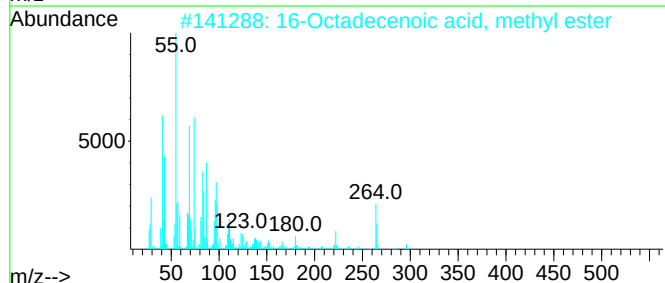
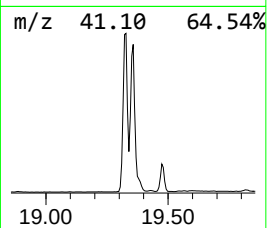
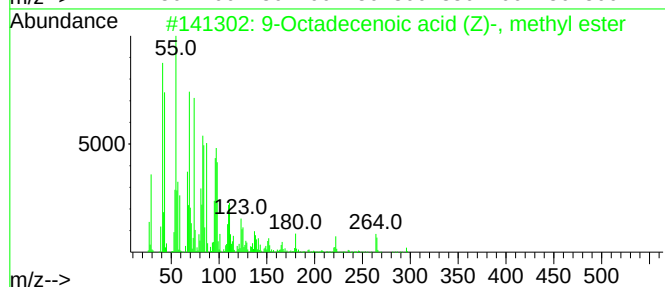
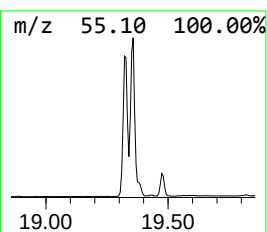
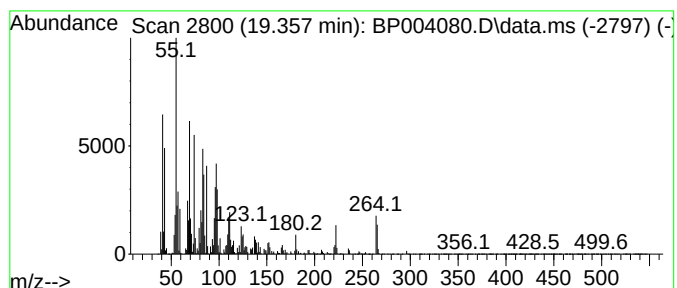
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.357	94.67 ng	7131530	Phenanthrene-d10	17.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99



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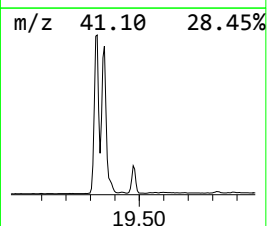
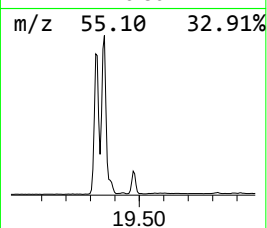
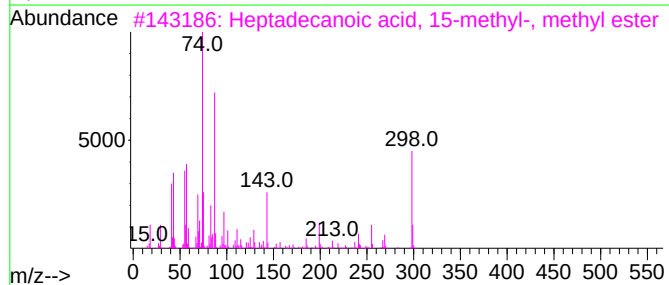
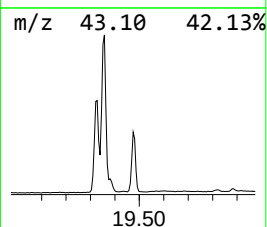
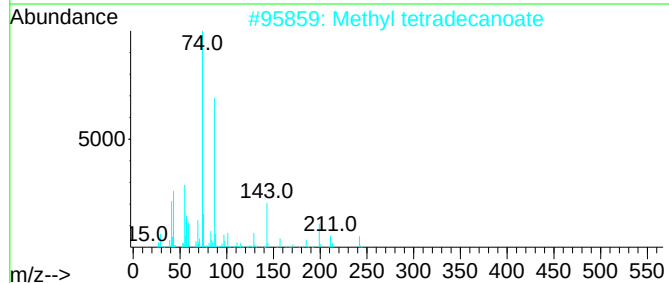
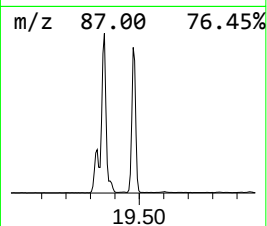
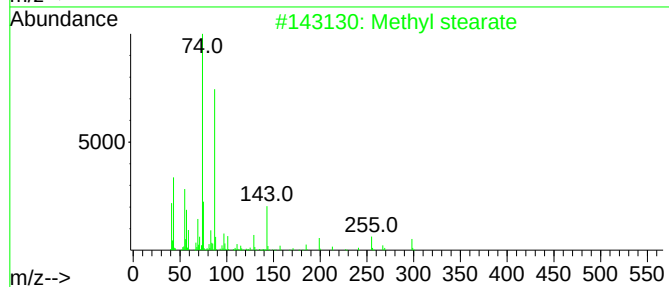
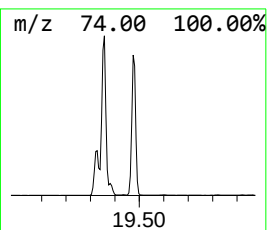
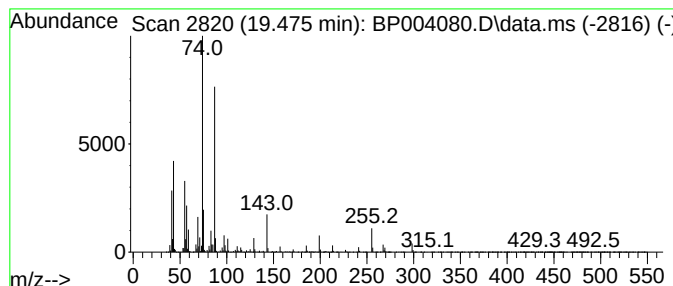
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.474	16.13 ng	1214810	Phenanthrene-d10	17.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	93
4			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112420\
Data File : BP004080.D
Acq On : 24 Nov 2020 17:35
Operator : CG/JU
Sample : L4597-01 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-112320

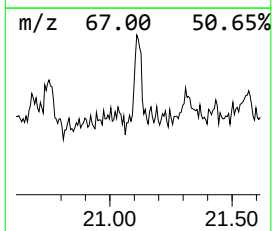
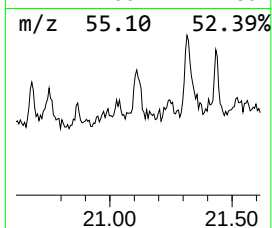
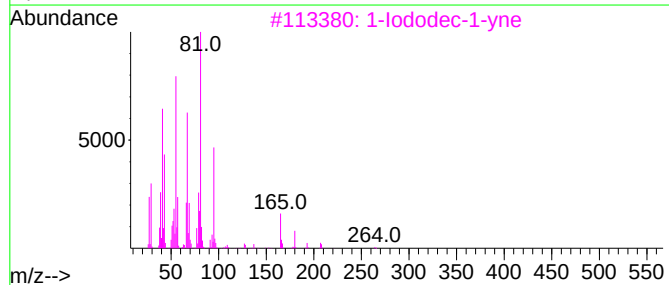
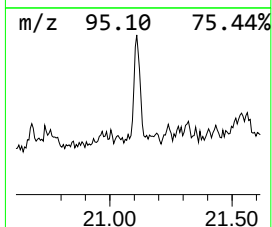
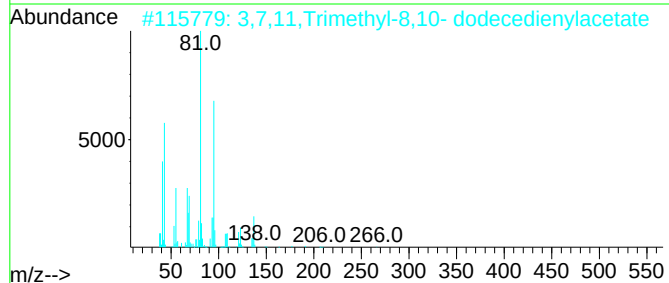
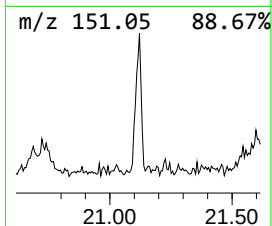
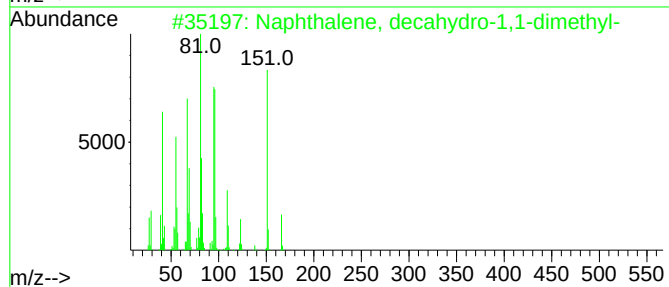
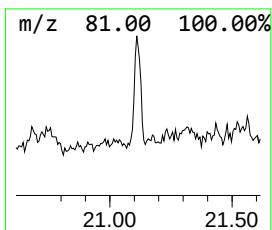
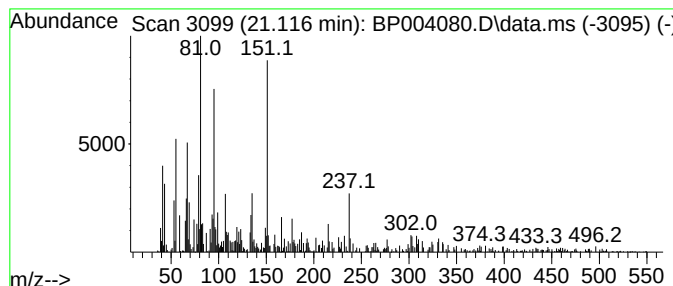
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Naphthalene, decahydro-1,1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.116	2.24 ng	162050	Chrysene-d12	21.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-1,1-dimet...	166	C12H22	035431-04-0	70
2			3,7,11,Trimethyl-8,10- dodecedie...	266	C17H30O2	1000374-10-3	60
3			1-Iododec-1-yne	264	C10H17I	067826-81-7	41
4			Stibine, triethyl-	208	C6H15Sb	000617-85-6	35
5			2-Furanone, 4-methyl-5-(1-butene...	206	C13H18O2	1000154-19-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112420\
Data File : BP004080.D
Acq On : 24 Nov 2020 17:35
Operator : CG/JU
Sample : L4597-01 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-112320

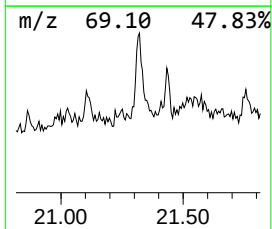
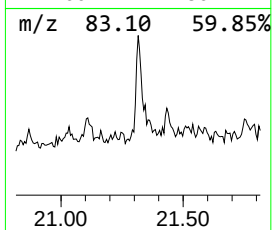
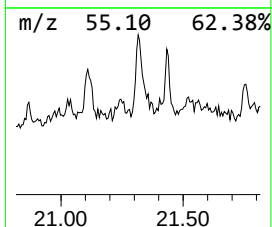
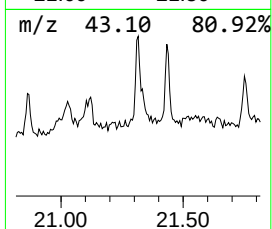
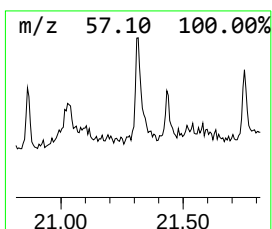
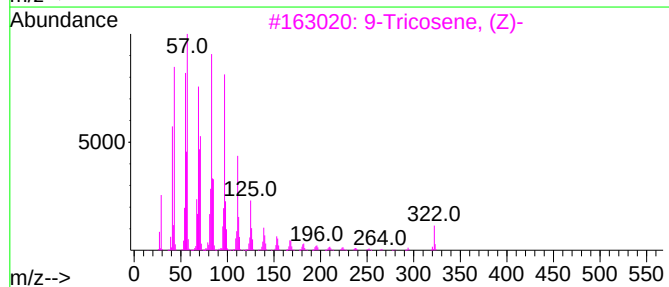
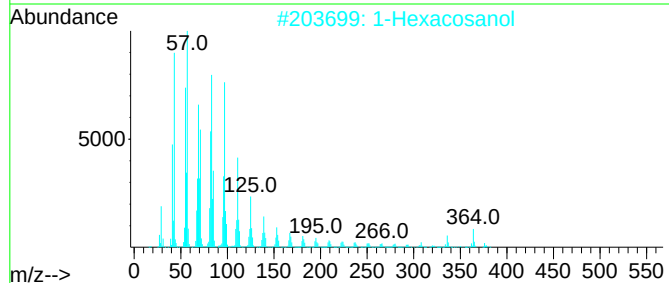
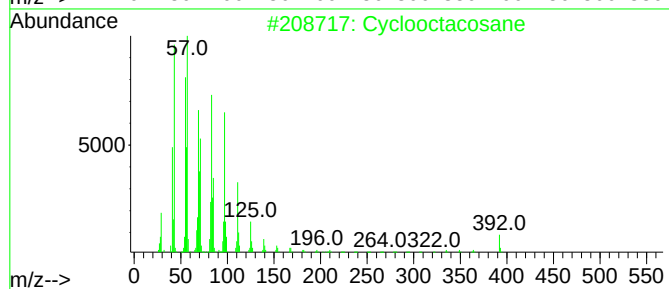
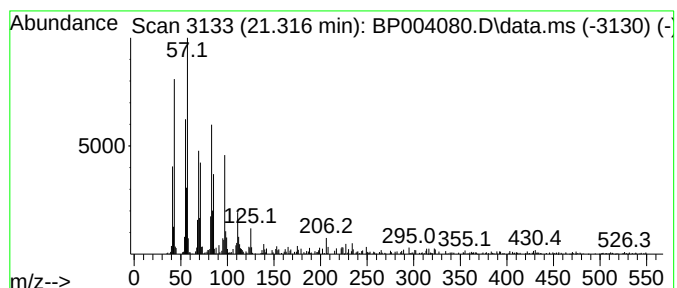
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclooctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.316	2.62 ng	189704	Chrysene-d12	21.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclooctacosane	392	C28H56	000297-24-5	94
2		1-Hexacosanol	382	C26H54O	000506-52-5	94
3		9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
4		Octadecane, 1-(ethenyl)-	296	C20H40	000930-02-9	91
5		11-Tricosene	322	C23H46	052078-56-5	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112420\
Data File : BP004080.D
Acq On : 24 Nov 2020 17:35
Operator : CG/JU
Sample : L4597-01 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BU-03-112320

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-di...	2.917	118.3	ng	4566580	1	8.263	771679	20.0
Butane, 2-metho...	3.164	4.5	ng	171839	1	8.263	771679	20.0
Hexadecanoic ac...	18.239	24.2	ng	1824330	4	17.628	1506530	20.0
9,12-Octadecadi...	19.328	107.9	ng	8126310	4	17.628	1506530	20.0
9-Octadecenoic ...	19.357	94.7	ng	7131530	4	17.628	1506530	20.0
Methyl stearate	19.474	16.1	ng	1214810	4	17.628	1506530	20.0
Naphthalene, de...	21.116	2.2	ng	162050	5	21.663	1445810	20.0
Cyclooctacosane	21.316	2.6	ng	189704	5	21.663	1445810	20.0