

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
 Data File : BP008828.D
 Acq On : 17 Jan 2022 17:35
 Operator : CG/JU
 Sample : N1144-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 RO-ETGI-352

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-BP011422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	7	11	31	rVB	2566541	3482875	20.58%	3.122%
2	5.434	410	416	434	rBV	4958323	7917086	46.78%	7.098%
3	7.028	678	687	705	rBV	4918688	8334907	49.25%	7.472%
4	7.852	818	827	835	rBV	1268644	2044991	12.08%	1.833%
5	9.010	1016	1024	1043	rBV	3037800	5323278	31.45%	4.772%
6	10.440	1259	1267	1279	rBV	231399	492277	2.91%	0.441%
7	10.651	1295	1303	1317	rBV	1658384	2893403	17.10%	2.594%
8	13.116	1714	1722	1737	rBV	8561099	12972305	76.65%	11.630%
9	14.492	1948	1956	1962	rBV	2531433	3936438	23.26%	3.529%
10	15.986	2203	2210	2230	rBV	7023742	10190531	60.21%	9.136%
11	17.245	2418	2424	2428	rBV	3258692	4626810	27.34%	4.148%
12	17.286	2428	2431	2437	rVB	866865	1192745	7.05%	1.069%
13	17.380	2443	2447	2453	rVB	203752	319999	1.89%	0.287%
14	17.927	2535	2540	2544	rBV	385645	470278	2.78%	0.422%
15	18.116	2568	2572	2574	rBV	192045	248210	1.47%	0.223%
16	18.151	2574	2578	2589	rVB2	452843	959785	5.67%	0.860%
17	18.304	2598	2604	2607	rBV2	291118	508875	3.01%	0.456%
18	18.339	2607	2610	2616	rVB	171148	231990	1.37%	0.208%
19	18.598	2650	2654	2658	rBV2	146869	207552	1.23%	0.186%
20	18.639	2658	2661	2672	rVB2	105130	207409	1.23%	0.186%
21	19.004	2719	2723	2727	rBV	225746	347707	2.05%	0.312%
22	19.057	2728	2732	2736	rVB3	518166	630523	3.73%	0.565%
23	19.139	2742	2746	2751	rBV	125288	213873	1.26%	0.192%
24	19.257	2761	2766	2774	rBV	2069320	2783803	16.45%	2.496%
25	19.610	2817	2826	2835	rBV	1830136	2956764	17.47%	2.651%
26	19.686	2836	2839	2844	rVB2	116108	187136	1.11%	0.168%
27	19.810	2855	2860	2865	rVB	14044904	16924791	100.00%	15.173%
28	20.092	2905	2908	2911	rVB	226646	247316	1.46%	0.222%
29	21.051	3068	3071	3079	rVB3	1126113	1478254	8.73%	1.325%
30	21.257	3102	3106	3110	rVB	917118	1029602	6.08%	0.923%
31	21.339	3114	3120	3124	rBV2	3356265	5389349	31.84%	4.831%
32	21.374	3124	3126	3135	rVB	729167	966938	5.71%	0.867%
33	21.457	3136	3140	3145	rBV	5062501	7033412	41.56%	6.305%
34	23.027	3403	3407	3412	rBV	757910	1365133	8.07%	1.224%
35	23.762	3527	3532	3539	rVB2	1792246	3429776	20.26%	3.075%

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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-BP011422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

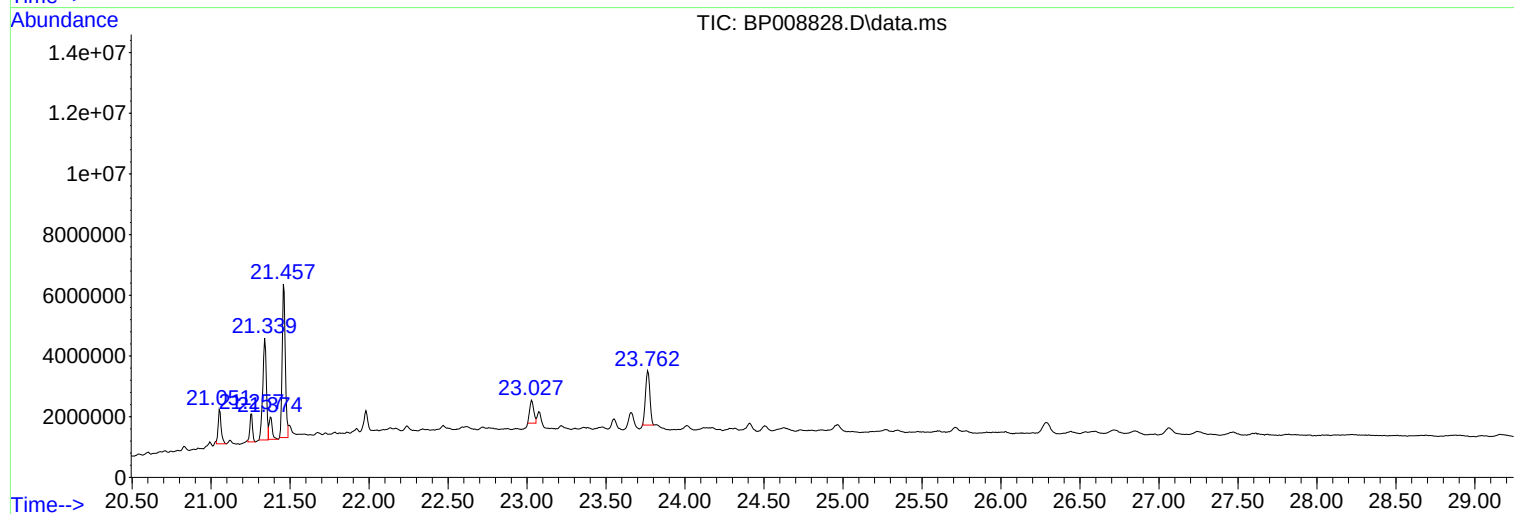
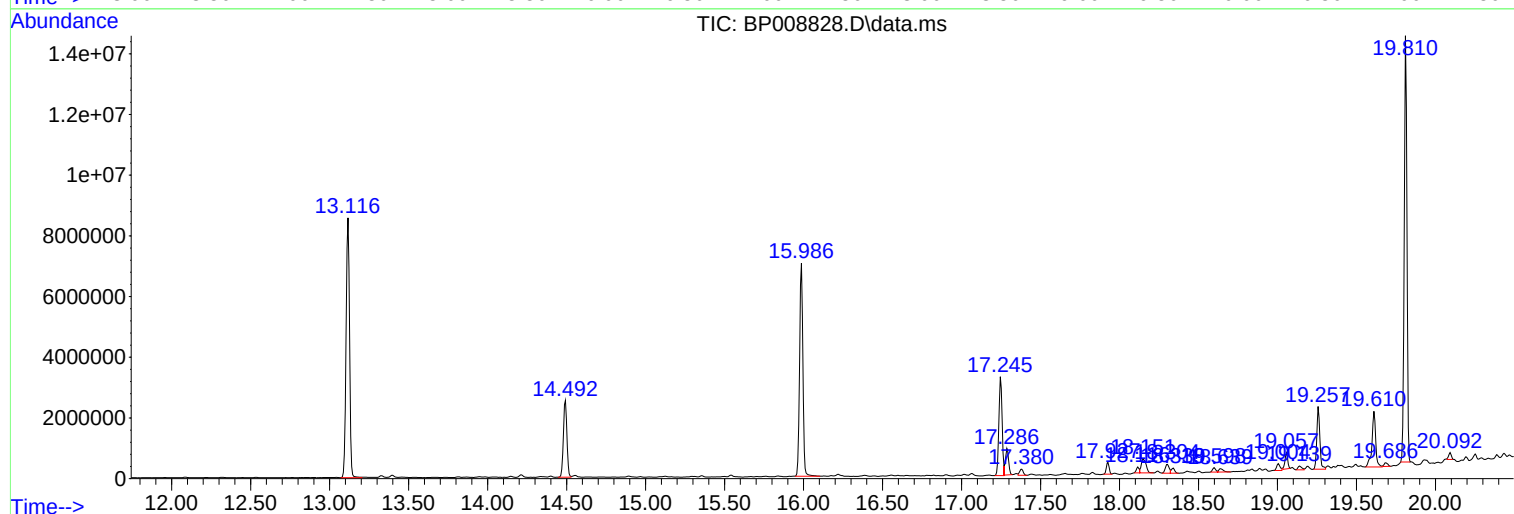
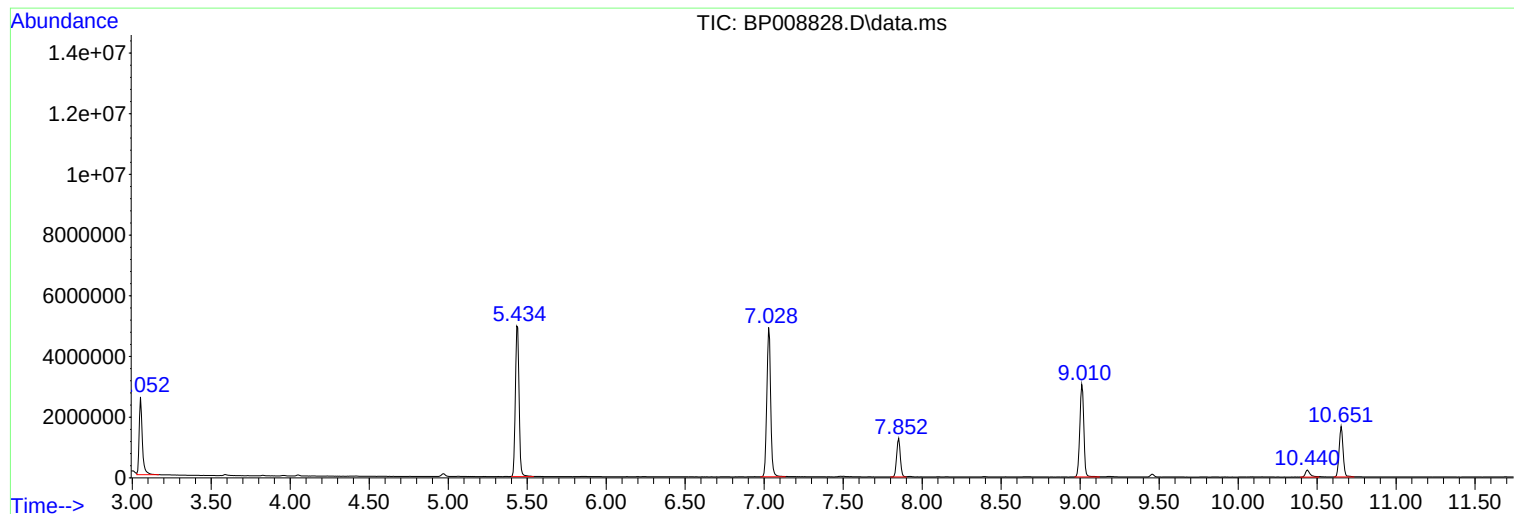
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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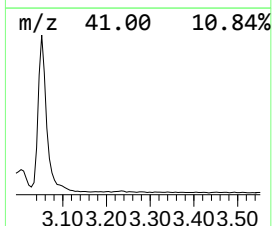
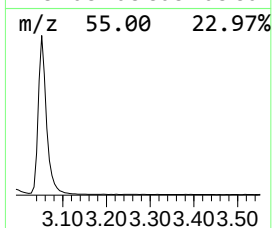
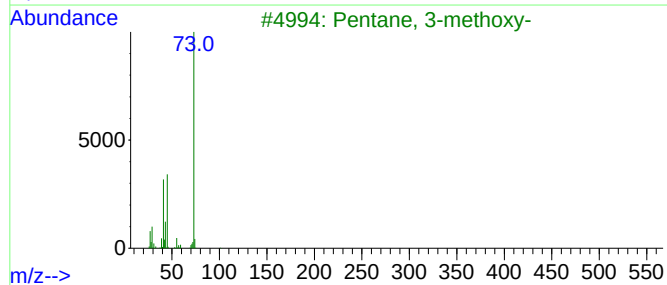
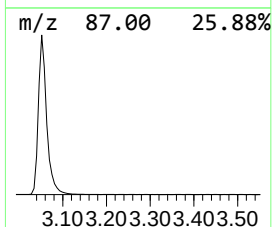
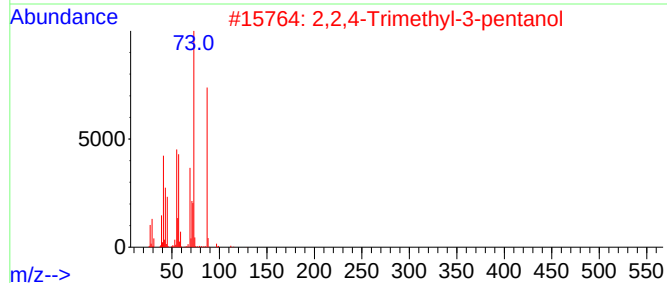
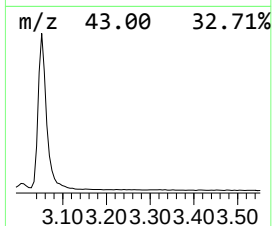
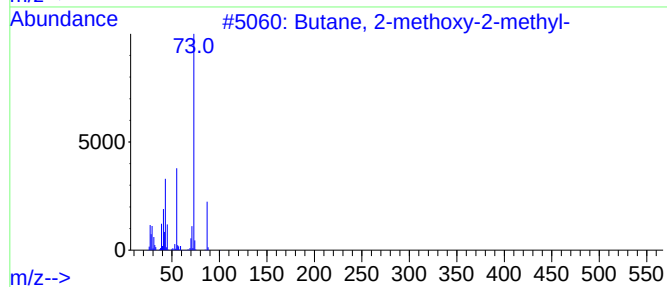
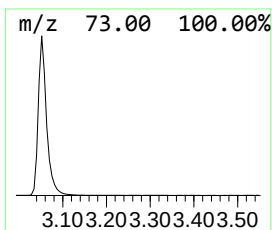
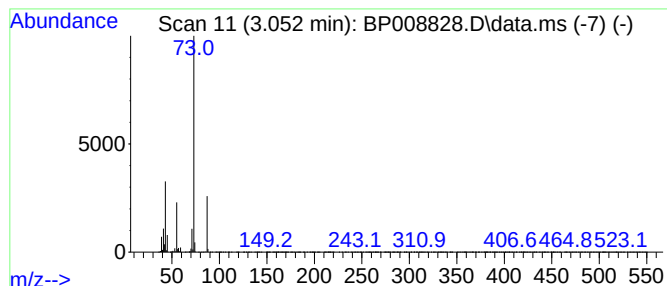
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	34.06 ng	3482880	1,4-Dichlorobenzene-d4	7.852

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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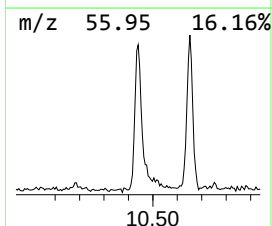
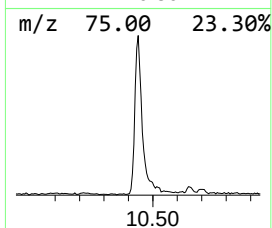
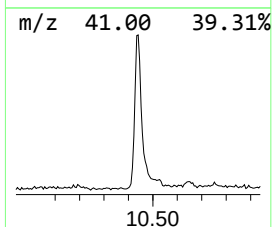
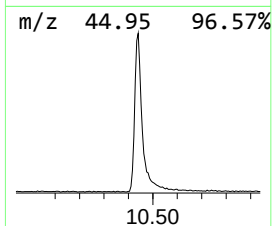
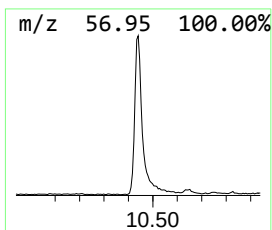
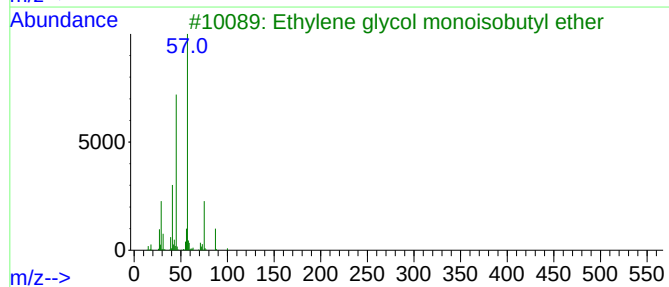
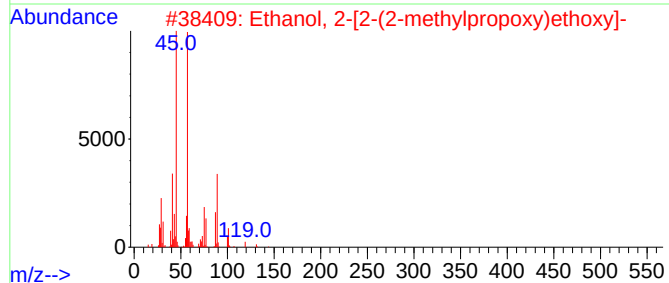
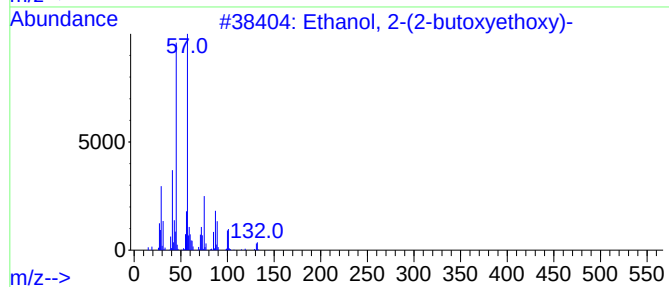
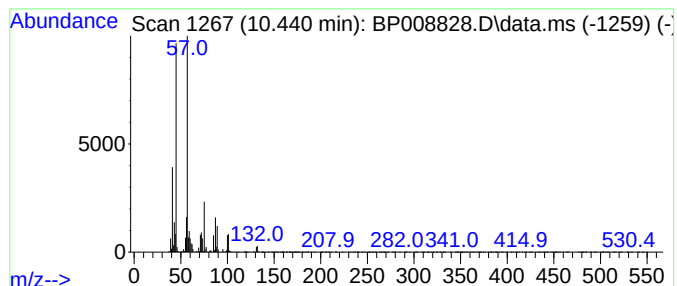
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.440	3.40 ng	492277	Naphthalene-d8	10.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	52
5			12-Crown-4	176	C8H16O4	000294-93-9	50



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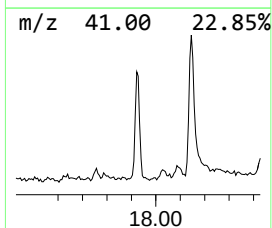
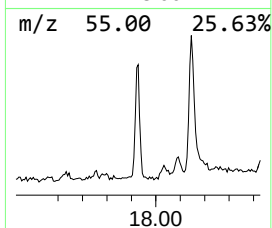
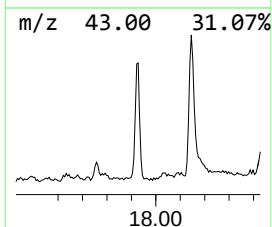
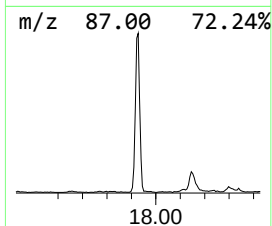
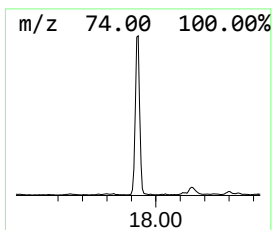
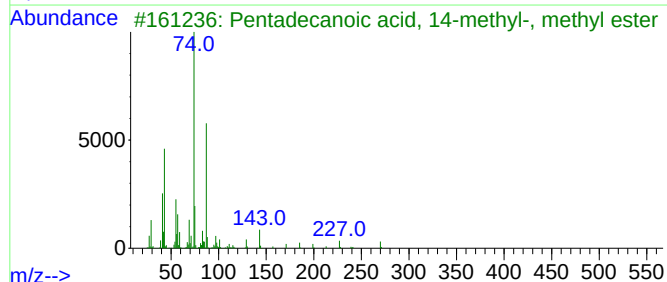
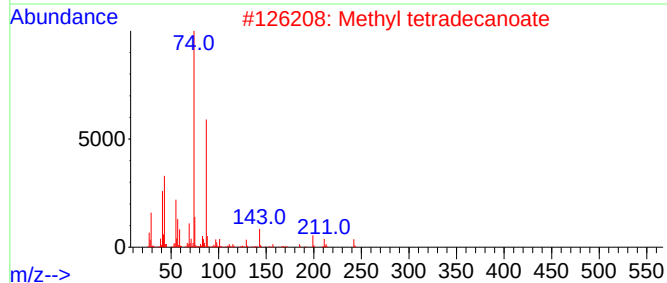
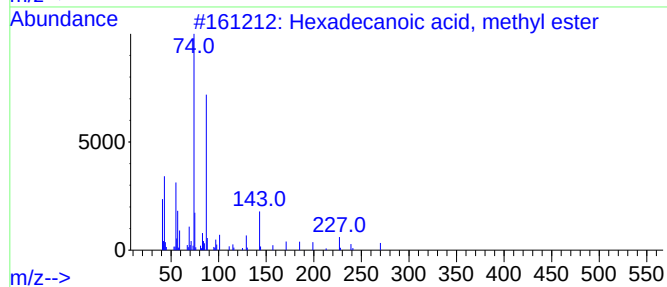
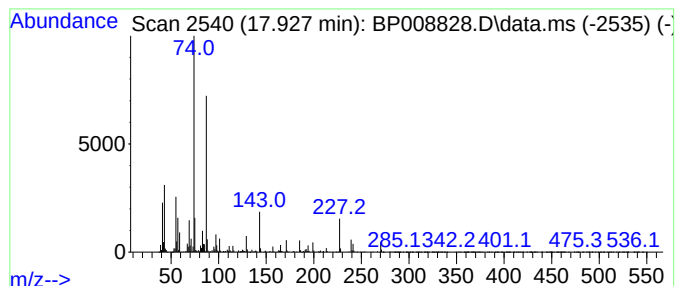
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.927	2.03 ng	470278	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	81
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80



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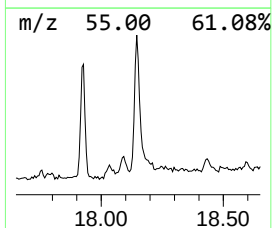
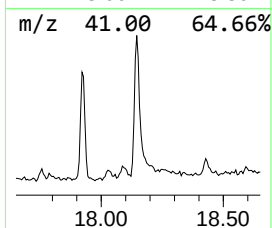
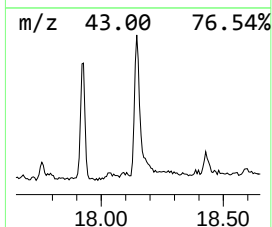
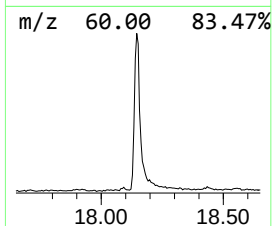
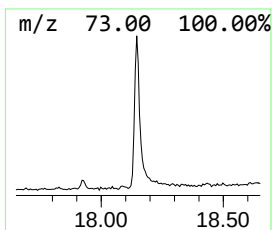
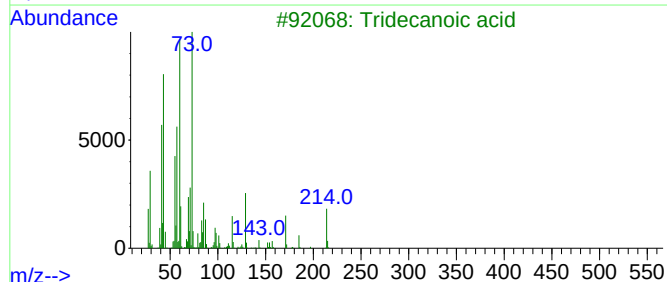
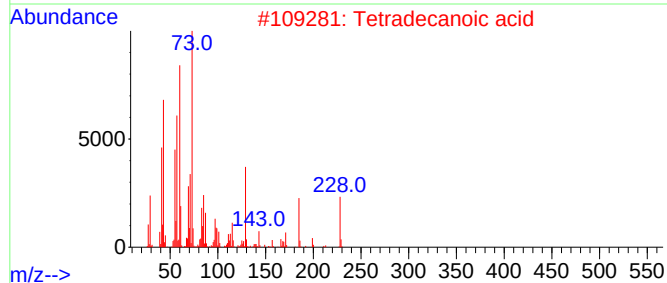
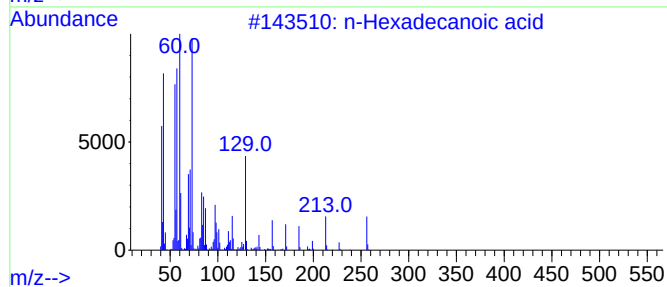
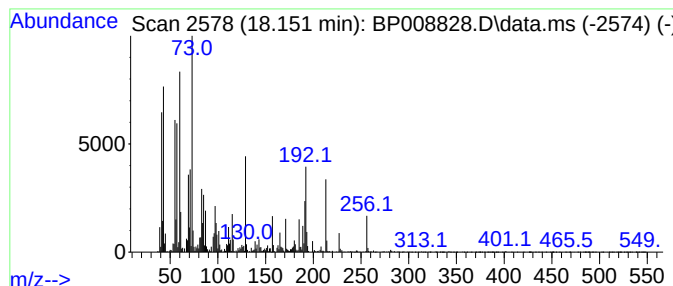
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	4.15 ng	959785	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Octadecanoic acid	284	C18H36O2	000057-11-4	64



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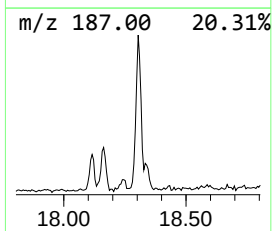
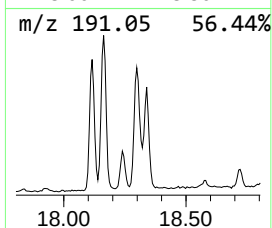
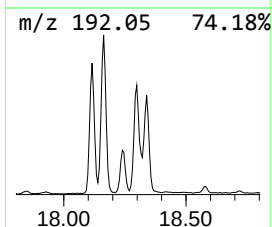
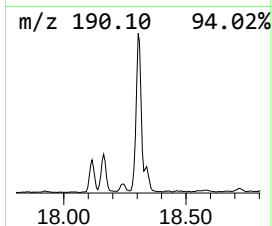
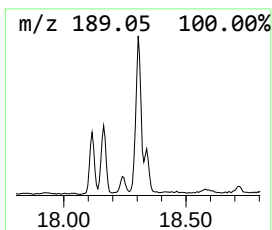
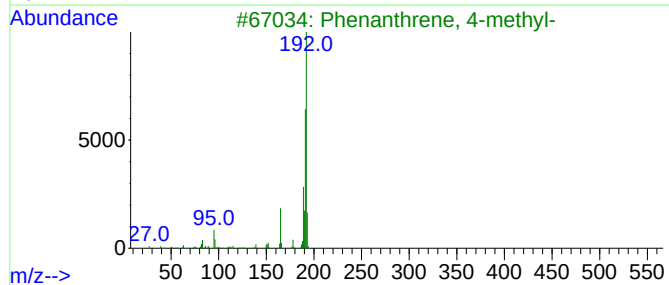
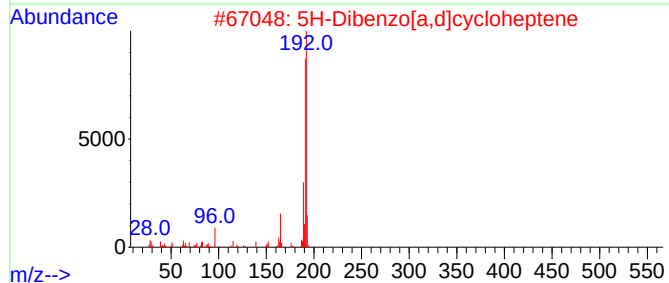
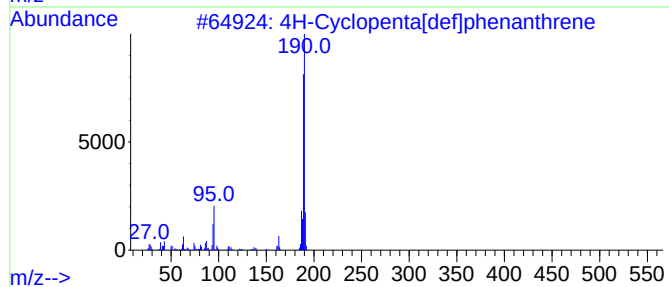
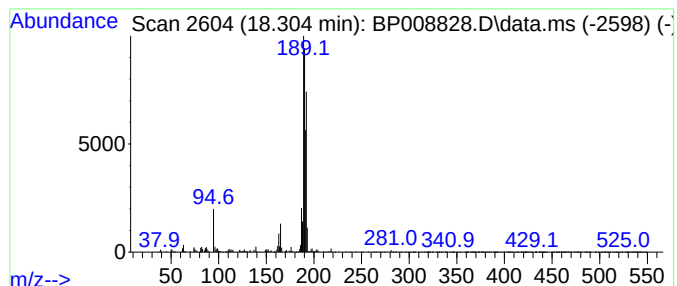
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown18.304 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.304	2.20 ng	508875	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
2			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
4			8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	38
5			Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008828.D
Acq On : 17 Jan 2022 17:35
Operator : CG/JU
Sample : N1144-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-ETGI-352

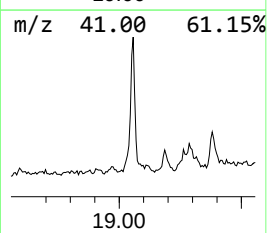
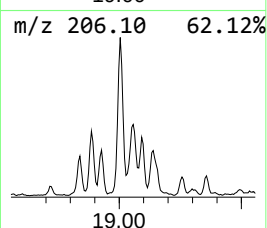
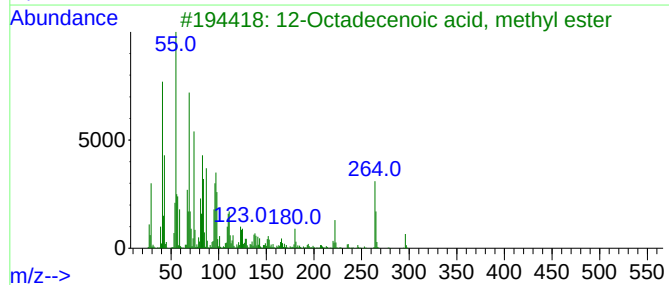
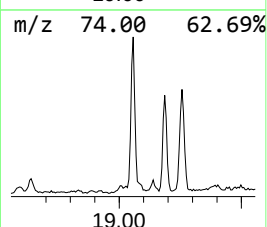
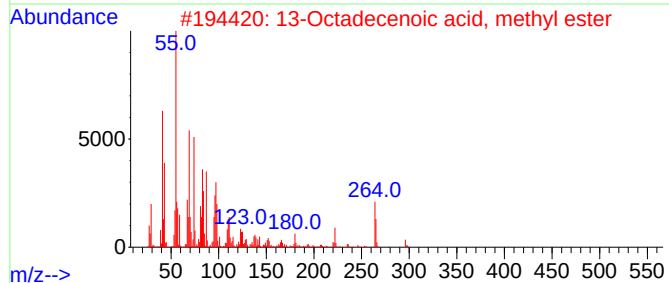
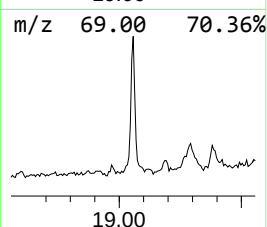
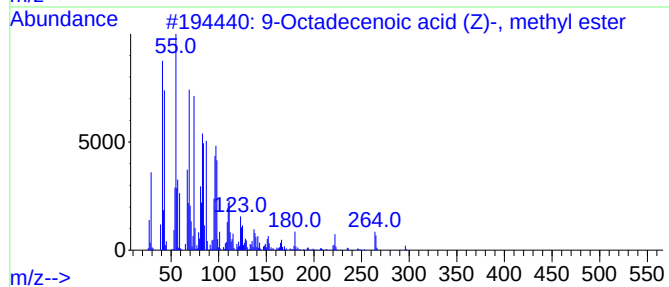
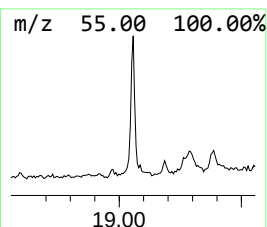
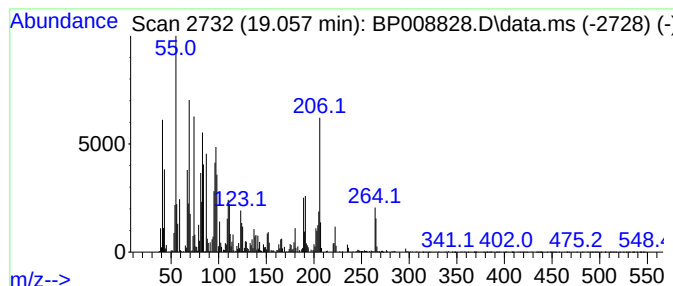
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.057	2.73 ng	630523	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
4			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
5			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008828.D
Acq On : 17 Jan 2022 17:35
Operator : CG/JU
Sample : N1144-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-ETGI-352

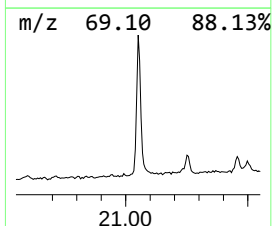
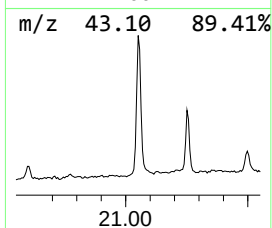
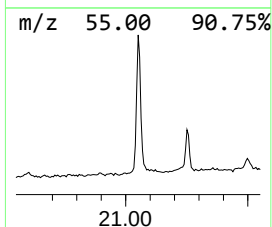
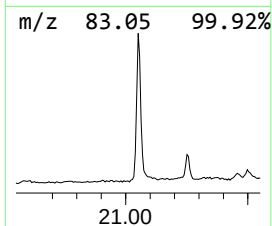
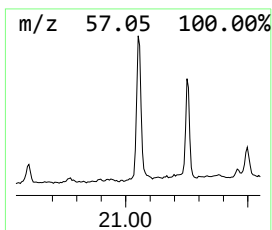
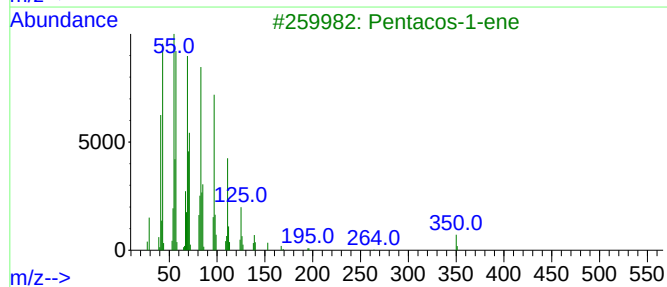
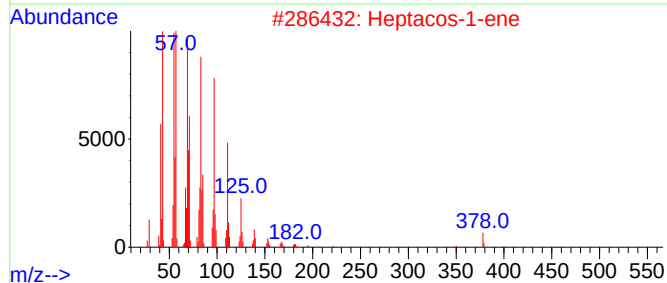
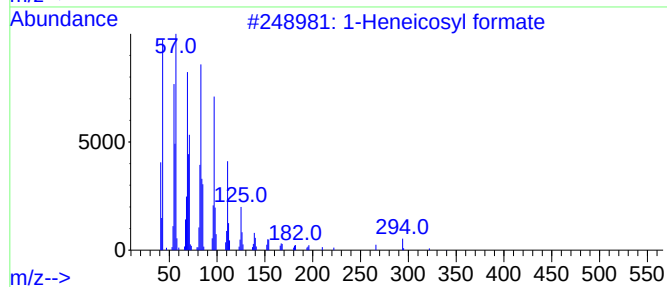
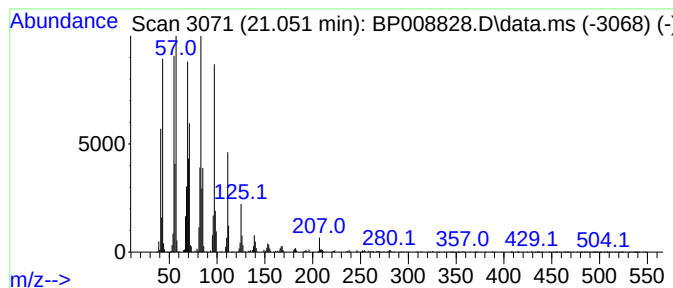
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	5.49 ng	1478250	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			Heptacos-1-ene	378	C27H54	015306-27-1	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			5-Octadecene, (E)-	252	C18H36	007206-21-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008828.D
Acq On : 17 Jan 2022 17:35
Operator : CG/JU
Sample : N1144-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-ETGI-352

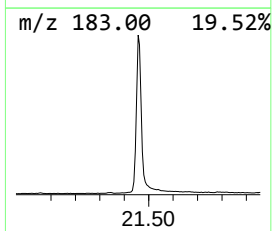
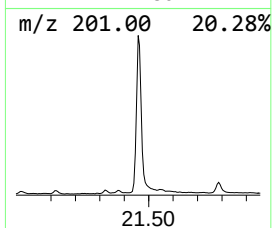
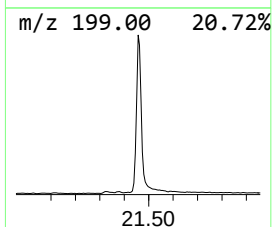
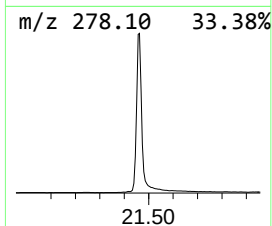
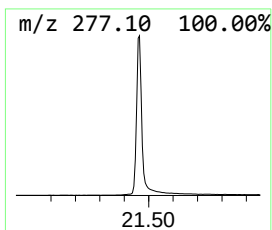
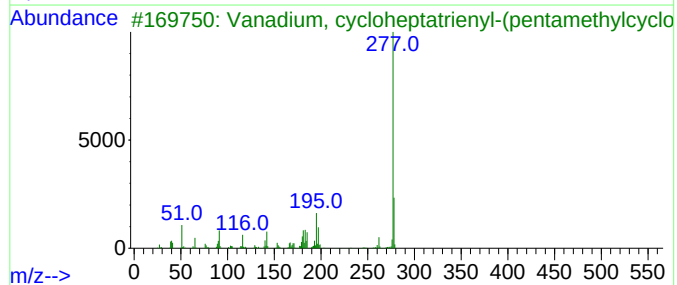
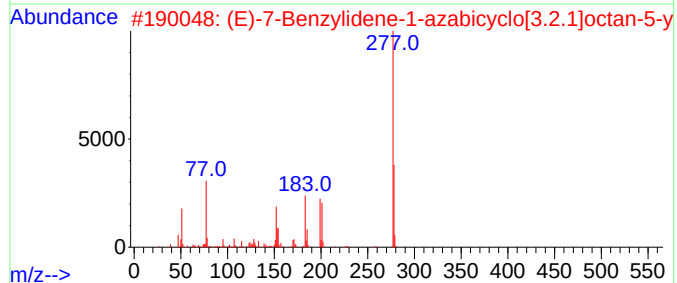
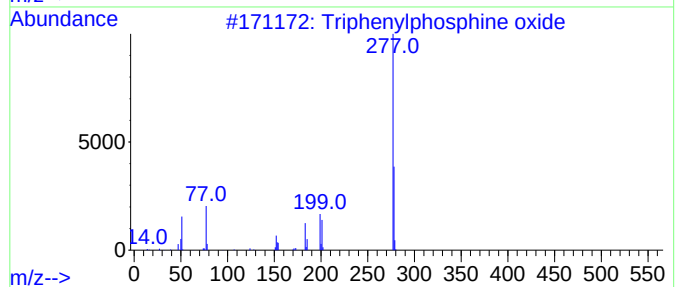
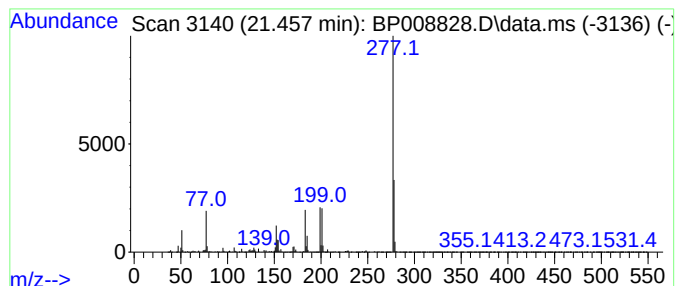
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.457	26.10 ng	7033410	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	90
3			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25
5			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008828.D
Acq On : 17 Jan 2022 17:35
Operator : CG/JU
Sample : N1144-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-ETGI-352

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.052	34.1	ng	3482880	1	7.852	2044990	20.0
Ethanol, 2-(2-b...	10.440	3.4	ng	492277	2	10.651	2893400	20.0
Hexadecanoic ac...	17.927	2.0	ng	470278	4	17.245	4626810	20.0
n-Hexadecanoic ...	18.151	4.2	ng	959785	4	17.245	4626810	20.0
unknown18.304	18.304	2.2	ng	508875	4	17.245	4626810	20.0
9-Octadecenoic ...	19.057	2.7	ng	630523	4	17.245	4626810	20.0
1-Heneicosyl fo...	21.051	5.5	ng	1478250	5	21.339	5389350	20.0
Triphenylphosph...	21.457	26.1	ng	7033410	5	21.339	5389350	20.0