

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022124\
 Data File : BP019812.D
 Acq On : 21 Feb 2024 17:28
 Operator : MA/JU
 Sample : P1537-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 4

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: BP019812.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.129	3	7	18	rVB	611686	739219	19.56%	3.718%
2	4.070	160	167	175	rVB3	42051	73745	1.95%	0.371%
3	4.305	202	207	217	rBV2	41912	72199	1.91%	0.363%
4	4.634	259	263	268	rBV	67288	101545	2.69%	0.511%
5	4.687	268	272	275	rBV	35742	54005	1.43%	0.272%
6	5.011	321	327	337	rBV	211239	315649	8.35%	1.587%
7	5.470	398	405	417	rBV	824960	1276469	33.77%	6.420%
8	6.093	502	511	517	rBV2	24193	61089	1.62%	0.307%
9	6.717	612	617	625	rBV8	19904	49041	1.30%	0.247%
10	7.064	669	676	684	rBV	769150	1257263	33.26%	6.323%
11	7.593	762	766	783	rVB5	15573	38581	1.02%	0.194%
12	7.893	810	817	824	rVB	257245	418234	11.07%	2.103%
13	9.064	1008	1016	1026	rBV	509959	864699	22.88%	4.349%
14	10.693	1285	1293	1306	rBV	299402	537556	14.22%	2.704%
15	13.152	1704	1711	1723	rBV	1302959	2092170	55.35%	10.522%
16	14.528	1938	1945	1953	rBV	474087	734217	19.43%	3.693%
17	16.022	2189	2199	2220	rBV	1267486	2032671	53.78%	10.223%
18	17.287	2405	2414	2419	rBV	616890	989808	26.19%	4.978%
19	17.328	2419	2421	2429	rVV	72339	98170	2.60%	0.494%
20	18.181	2558	2566	2576	rBV2	394971	595233	15.75%	2.994%
21	18.339	2588	2593	2597	rBV3	29481	56482	1.49%	0.284%
22	19.292	2750	2755	2763	rBV	202688	290939	7.70%	1.463%
23	19.416	2772	2776	2785	rVB2	146554	192145	5.08%	0.966%
24	19.645	2807	2815	2823	rBV	196712	317865	8.41%	1.599%
25	19.851	2844	2850	2862	rBV	3032398	3779641	100.00%	19.009%
26	20.128	2895	2897	2901	rVB2	38012	43169	1.14%	0.217%
27	21.098	3058	3062	3068	rBV2	217464	272140	7.20%	1.369%
28	21.375	3103	3109	3114	rBV	928502	1377077	36.43%	6.926%
29	23.792	3514	3520	3529	rBV	572201	1152649	30.50%	5.797%

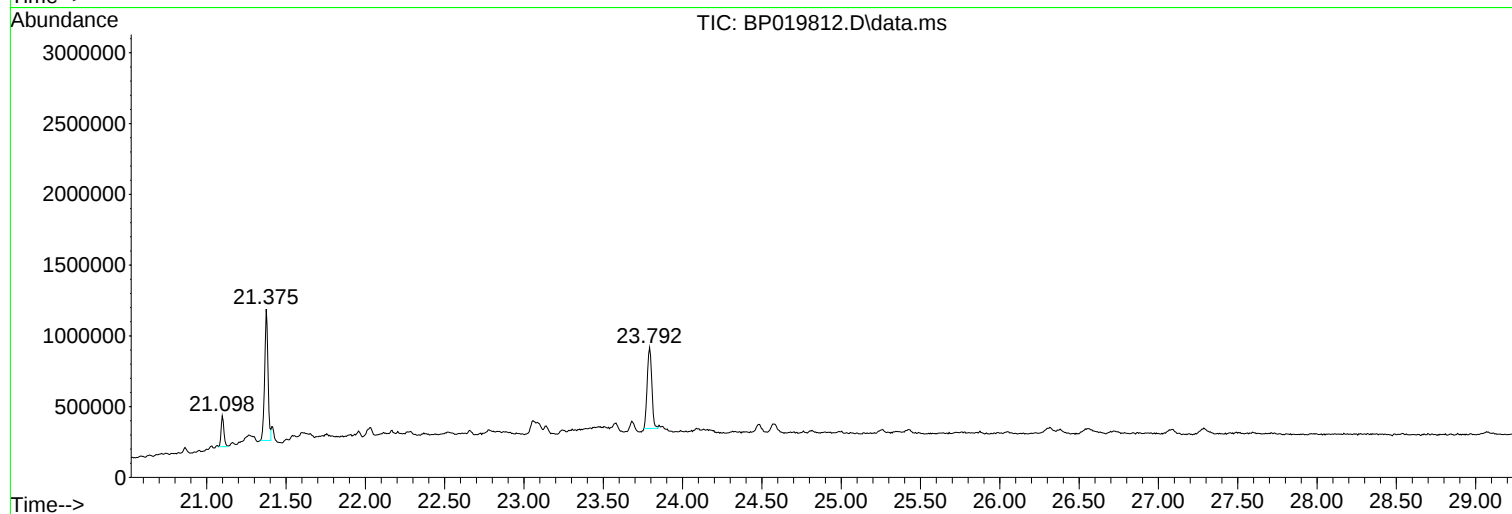
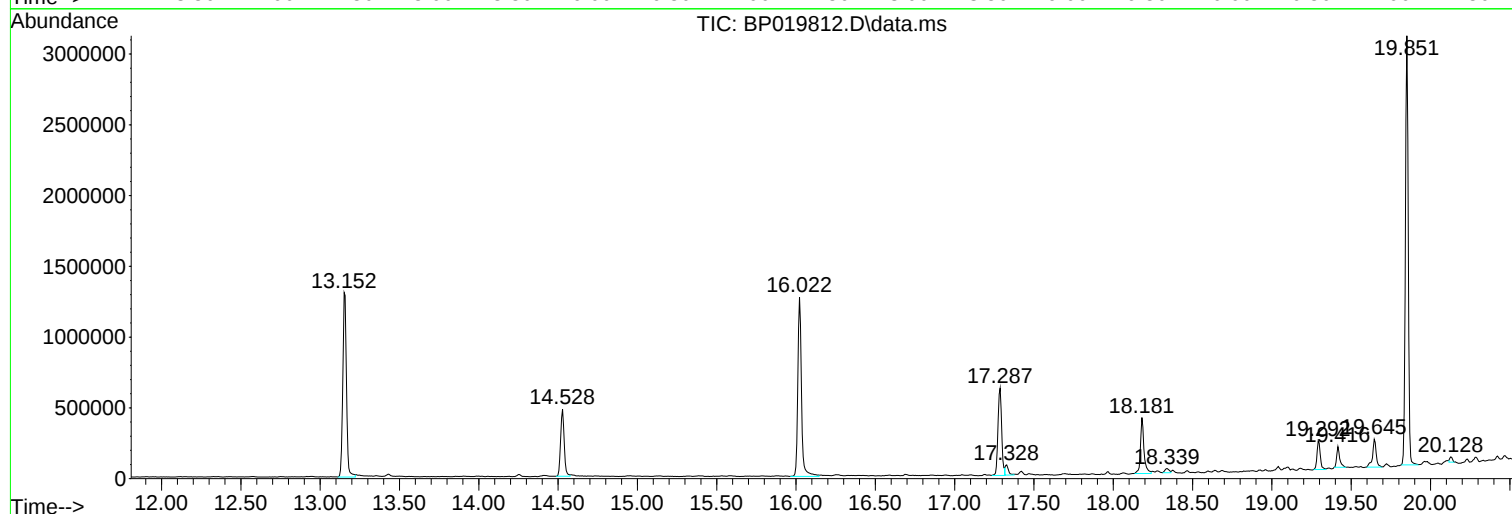
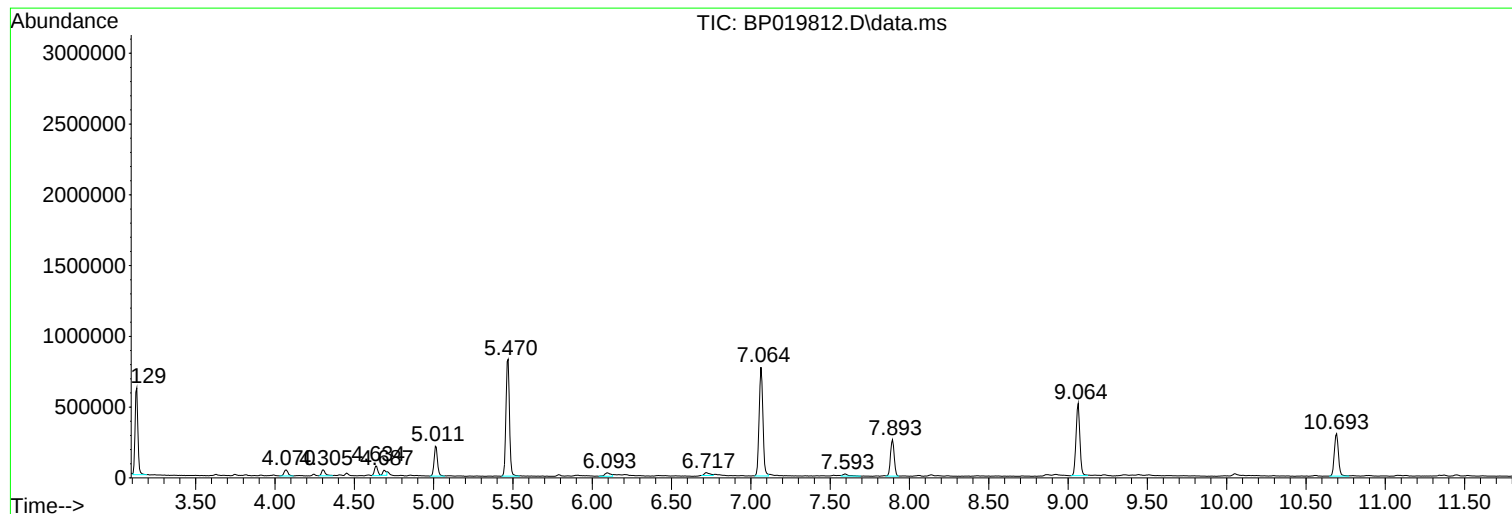
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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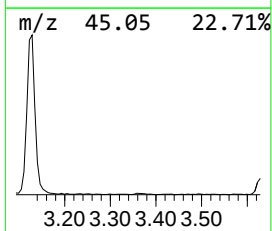
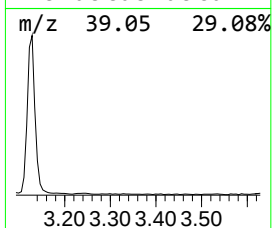
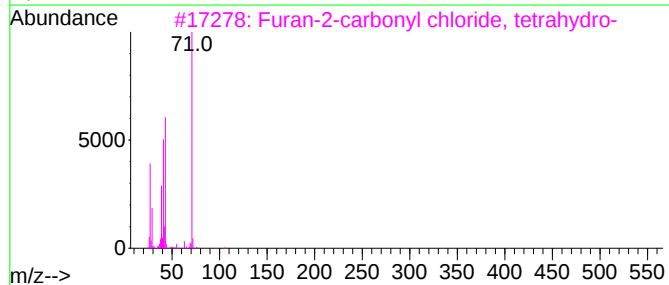
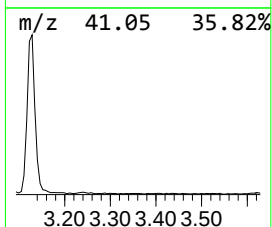
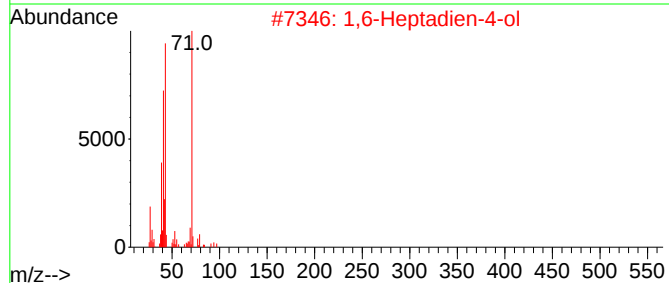
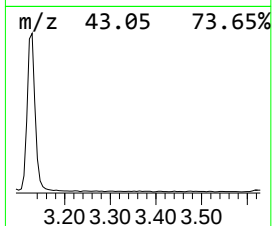
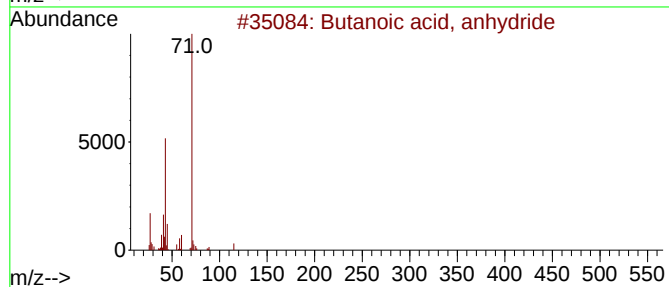
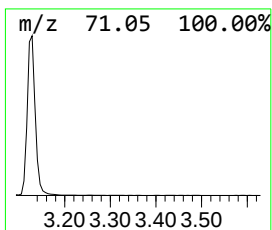
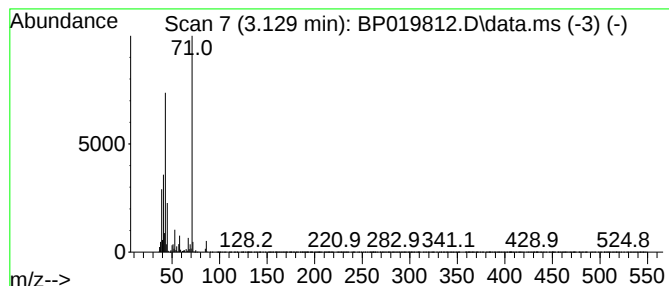
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid, anhydride Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.129	35.35 ng	739219	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	64
2			1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	59
3			Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	53
4			3-Penten-2-ol	86	C5H10O	001569-50-2	53
5			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	50



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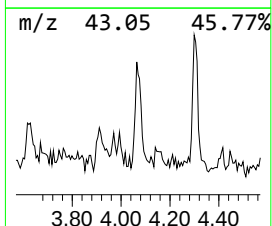
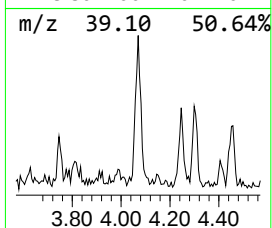
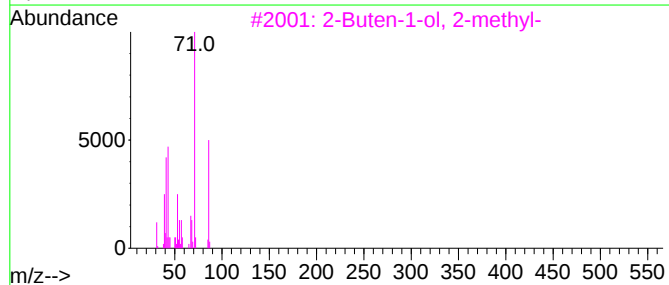
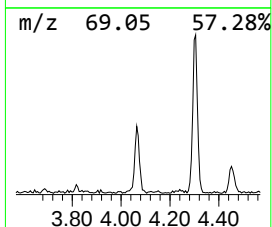
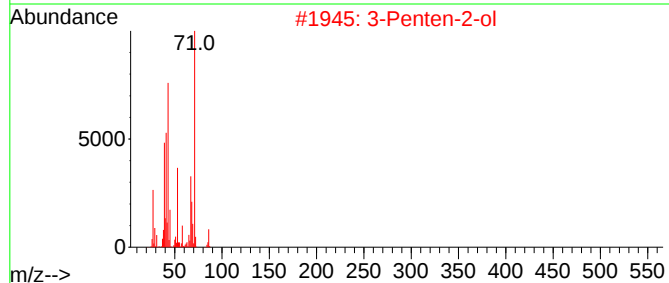
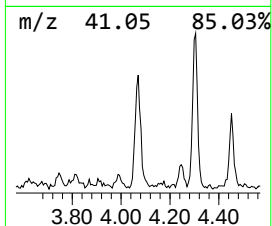
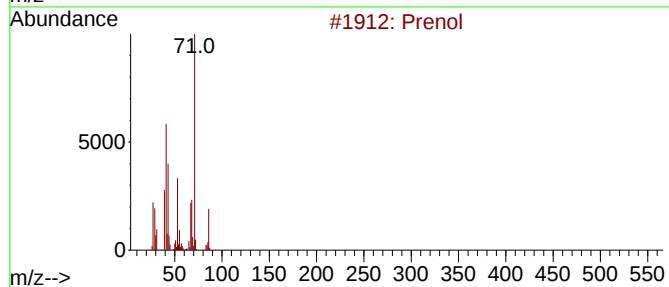
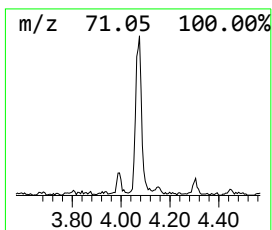
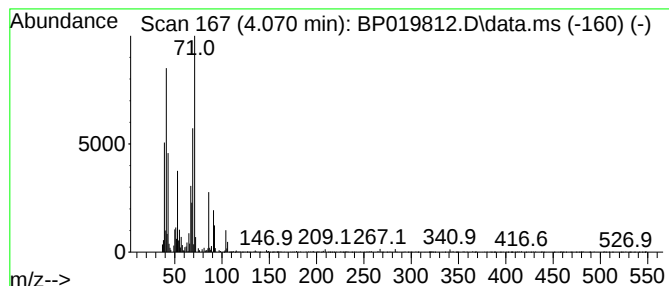
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Prenol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.070	3.53 ng	73745	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prenol	86	C5H10O	000556-82-1	58
2	3-Penten-2-ol	86	C5H10O	001569-50-2	50
3	2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	47
4	trans-1-Methoxy-1-butene	86	C5H10O	010034-13-6	38
5	3-Methoxybut-1-ene	86	C5H10O	017351-24-5	35



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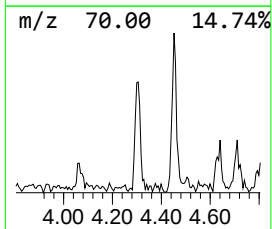
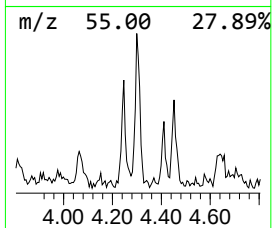
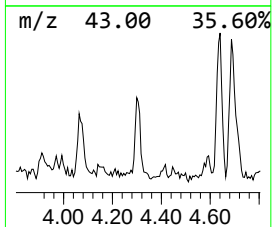
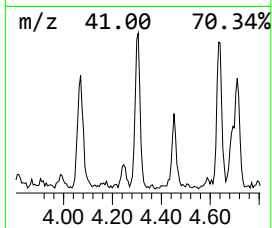
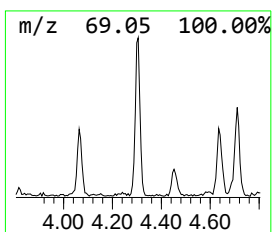
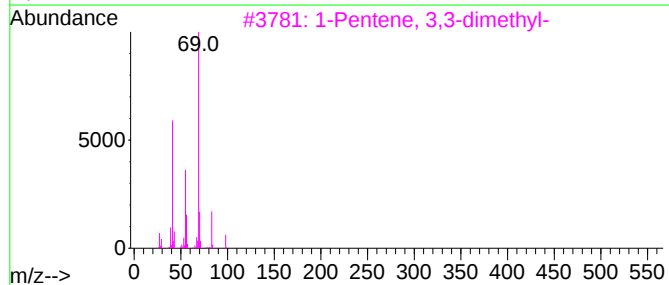
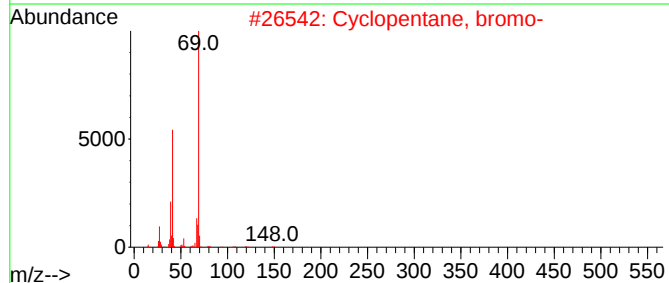
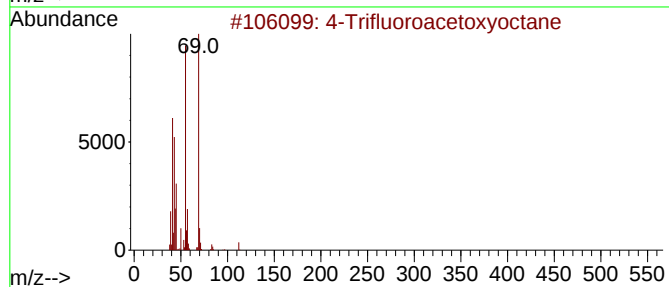
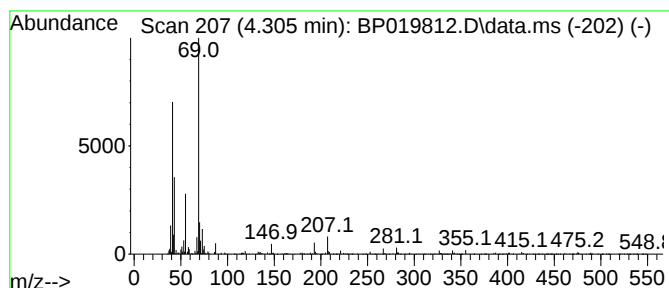
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-Trifluoroacetoxyoctane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.305	3.45 ng	72199	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Trifluoroacetoxyoctane	226	C10H17F3O2	116465-17-9	53
2			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	36
3			1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	36
4			1,5-Heptadiene, 2,3,6-trimethyl-	138	C10H18	033501-88-1	36
5			1-Pentyn-3-ol, 3-methyl-	98	C6H10O	000077-75-8	36



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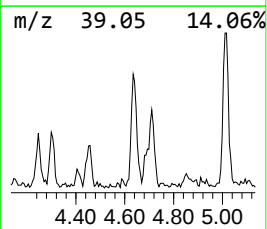
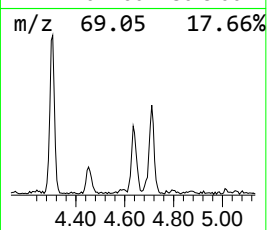
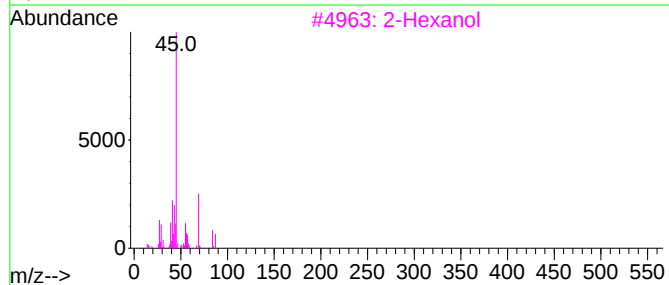
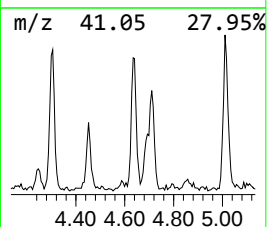
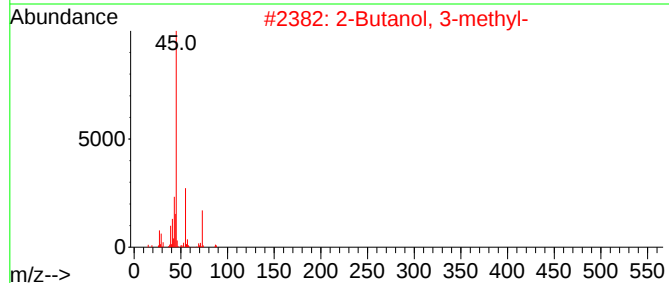
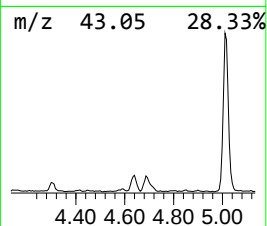
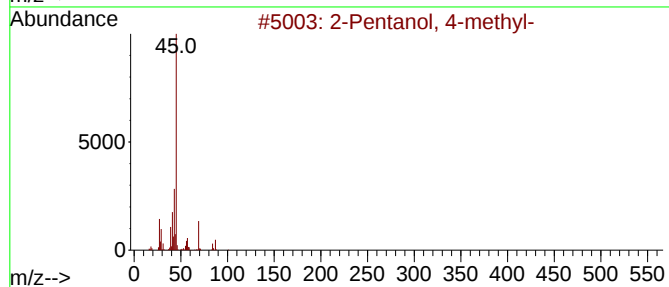
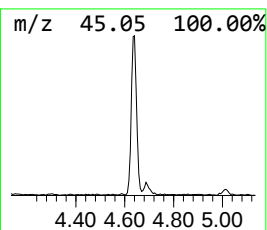
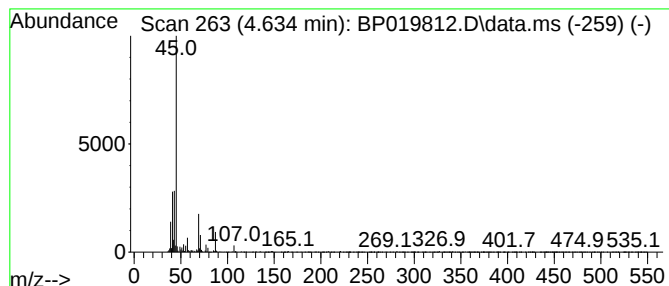
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Peak Number 4 2-Pentanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.634	4.86 ng	101545	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	72
2			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	59
3			2-Hexanol	102	C6H14O	000626-93-7	56
4			(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	53
5			Propanenitrile, 3-methoxy-	85	C4H7NO	000110-67-8	42



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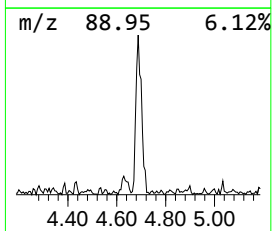
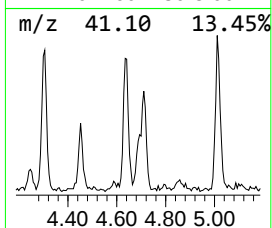
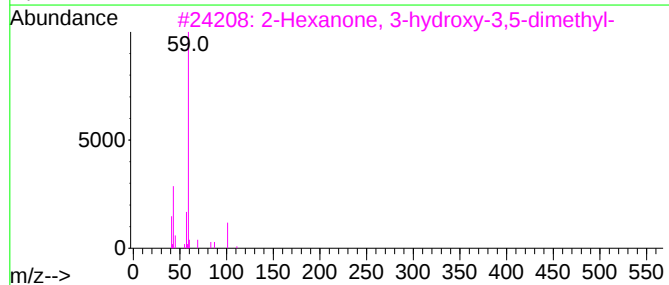
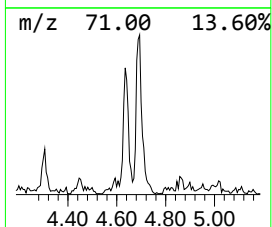
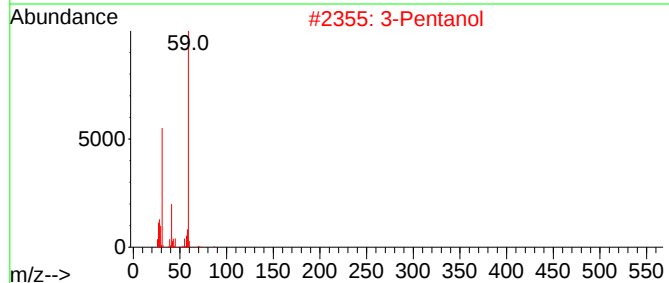
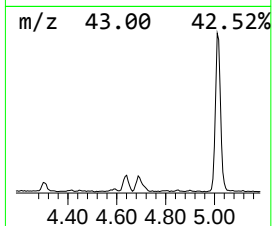
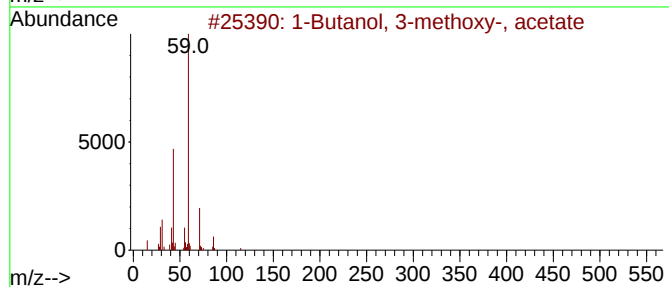
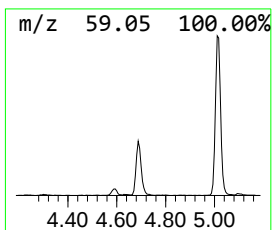
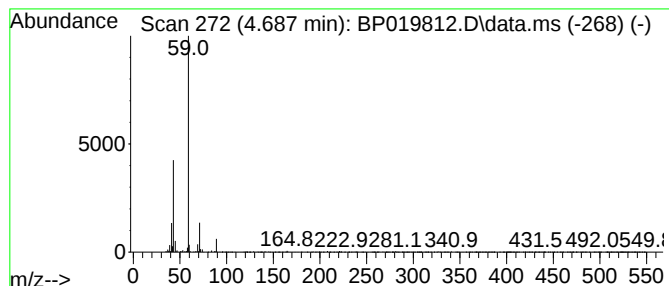
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Butanol, 3-methoxy-, acetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.687	2.58 ng	54005	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol, 3-methoxy-, acetate	146	C7H14O3	004435-53-4	50
2			3-Pentanol	88	C5H12O	000584-02-1	42
3			2-Hexanone, 3-hydroxy-3,5-dimethyl-	144	C8H16O2	006321-14-8	38
4			Tetraglyme	222	C10H22O5	000143-24-8	9
5			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9



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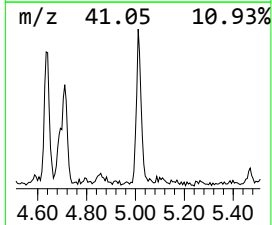
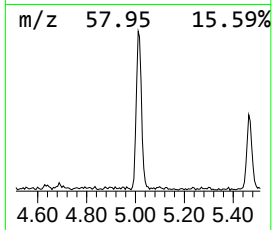
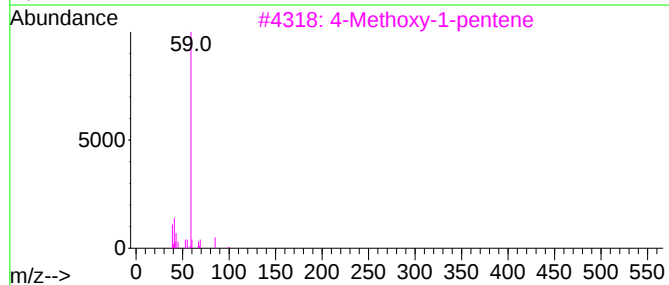
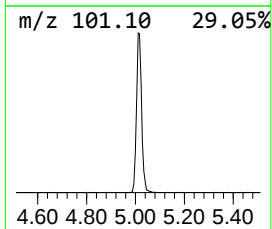
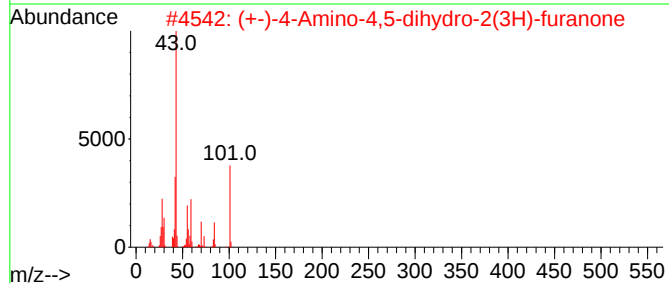
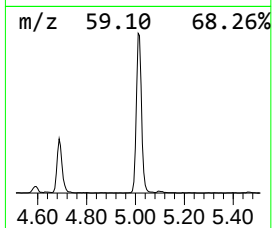
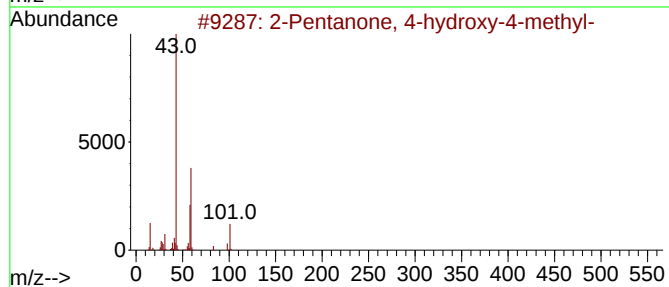
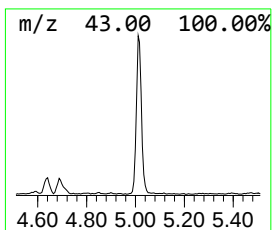
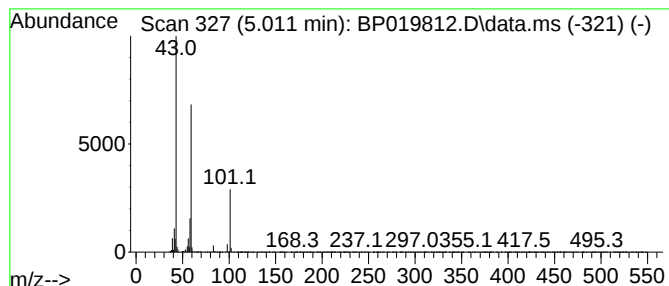
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.011	15.09 ng	315649	1,4-Dichlorobenzene-d4	7.893

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	43
3			4-Methoxy-1-pentene	100	C6H12O	098386-09-5	35
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022124\
Data File : BP019812.D
Acq On : 21 Feb 2024 17:28
Operator : MA/JU
Sample : P1537-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

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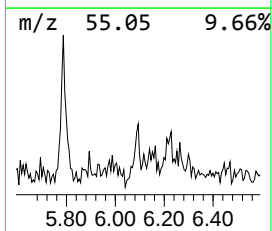
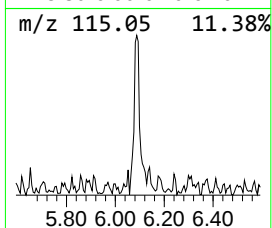
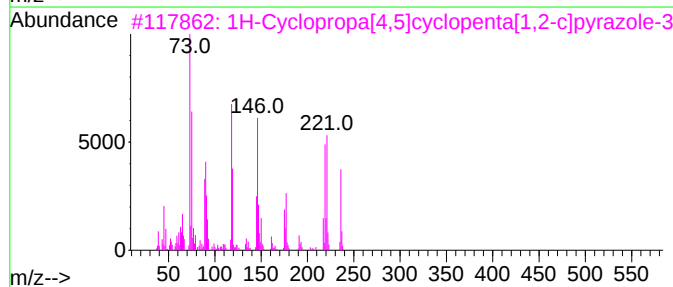
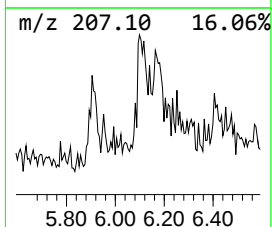
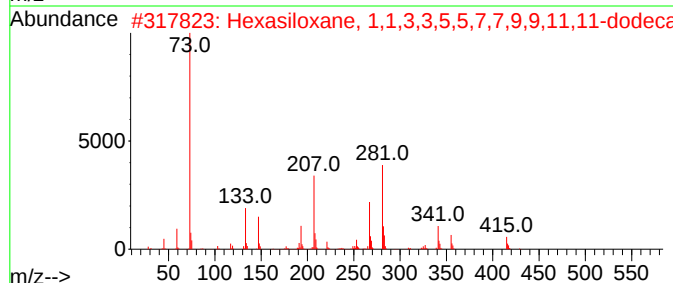
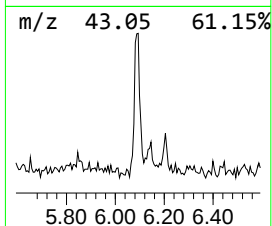
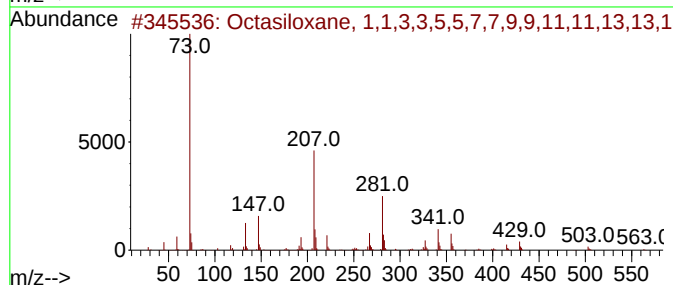
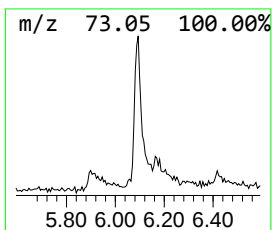
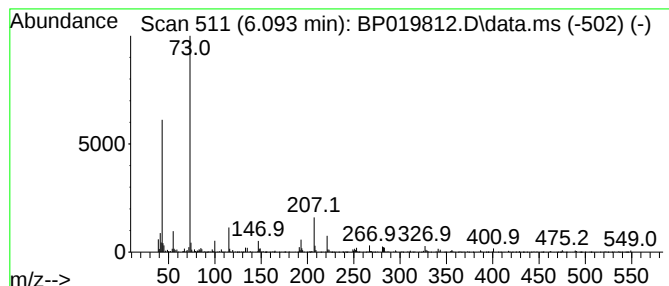
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.093 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.093	2.92 ng	61089	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H5007Si8	019095-24-0	38
2			Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H3805Si6	000995-82-4	38
3			1H-Cyclopropa[4,5]cyclopenta[1,2...	236	C11H16N2O2Si	1000499-60-1	27
4			Trenbolone, TMS	342	C21H3002Si	1034684-28-0	27
5			2-Pentanone, 4-methoxy-4-methyl-	130	C7H1402	000107-70-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022124\
Data File : BP019812.D
Acq On : 21 Feb 2024 17:28
Operator : MA/JU
Sample : P1537-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

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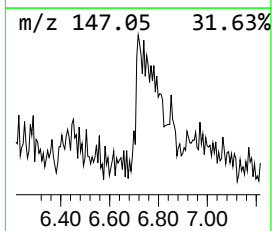
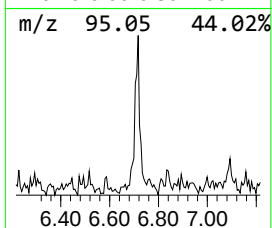
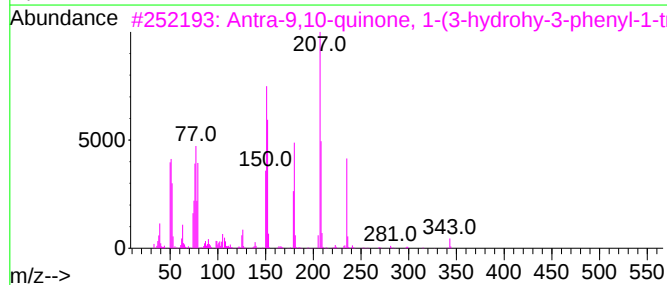
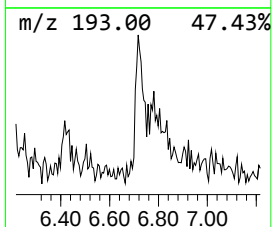
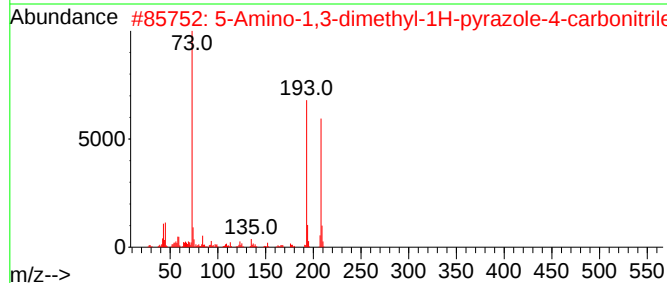
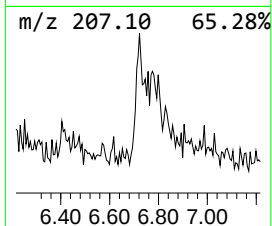
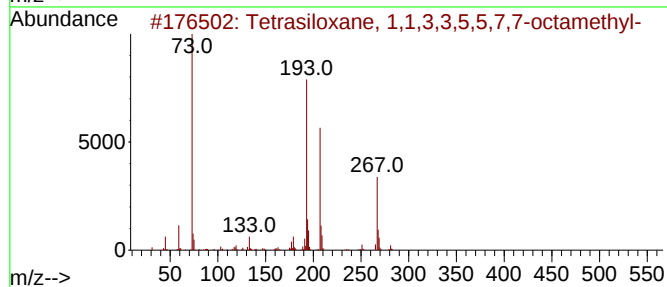
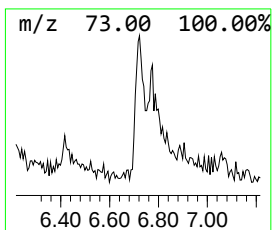
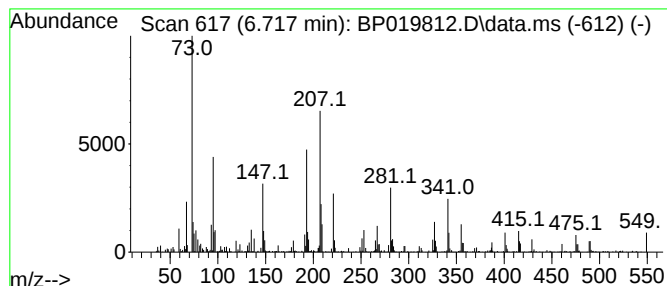
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown6.717 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.717	2.35 ng	49041	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrasiloxane, 1,1,3,3,5,5,7,7-o...	282	C8H26O3Si4	001000-05-1	16
2			5-Amino-1,3-dimethyl-1H-pyrazole...	208	C9H16N4Si	1000479-00-2	14
3			Antra-9,10-quinone, 1-(3-hydroxy...	343	C20H13N3O3	098496-82-3	11
4			3-Phenyllactic acid, 2TMS deriva...	310	C15H26O3Si2	027750-45-4	11
5			Formic acid, 1-(4,7-dihydro-2-me...	207	C9H9N3O3	1010267-28-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022124\
Data File : BP019812.D
Acq On : 21 Feb 2024 17:28
Operator : MA/JU
Sample : P1537-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

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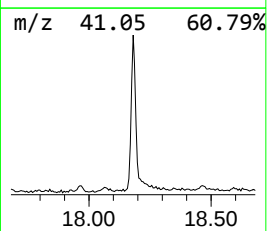
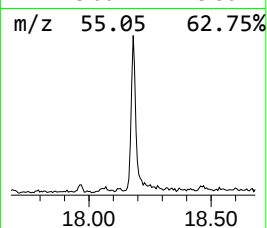
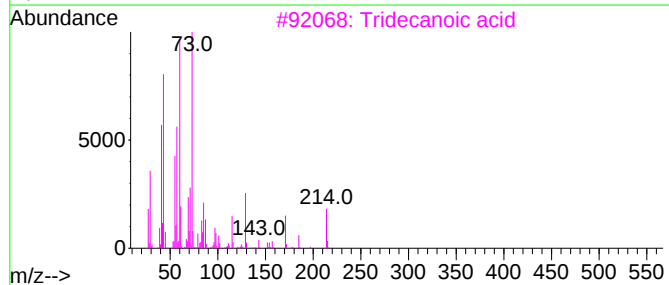
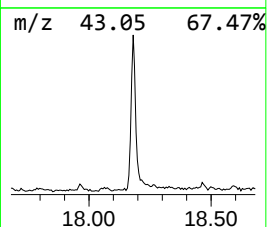
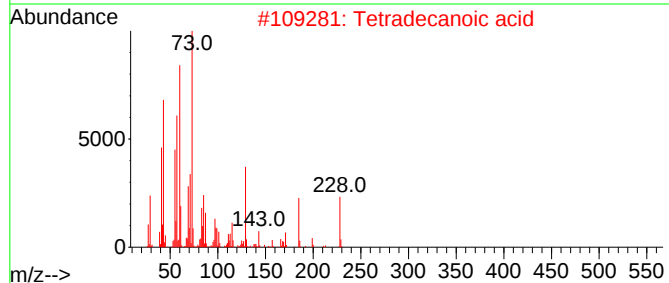
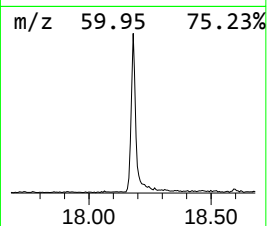
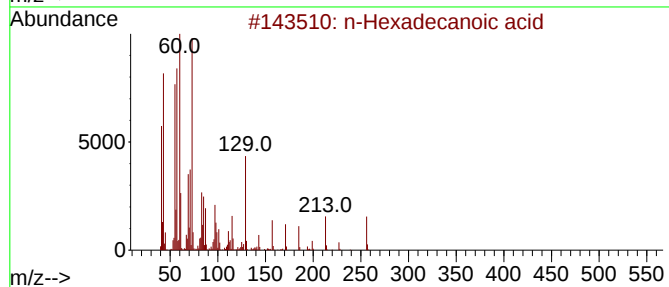
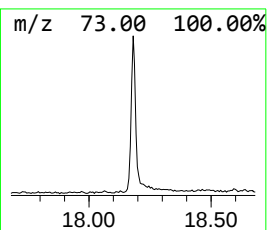
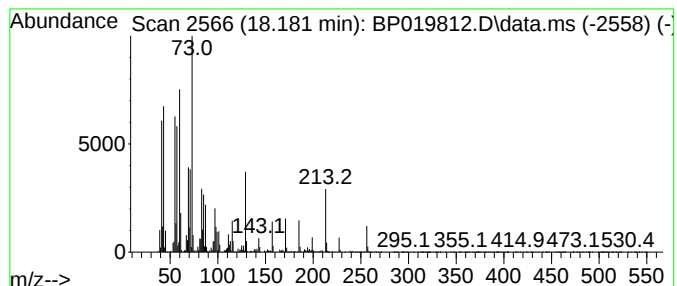
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.181	12.03 ng	595233	Phenanthrene-d10	17.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022124\
Data File : BP019812.D
Acq On : 21 Feb 2024 17:28
Operator : MA/JU
Sample : P1537-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

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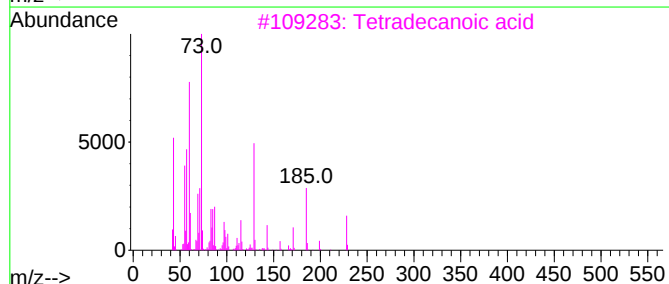
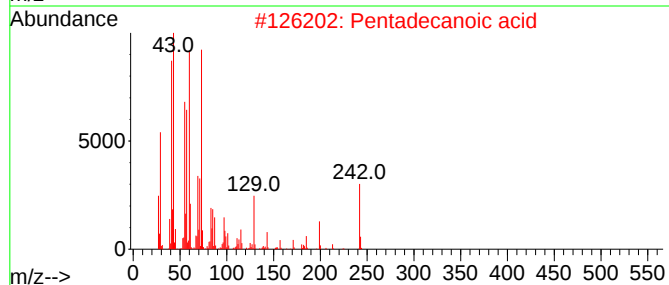
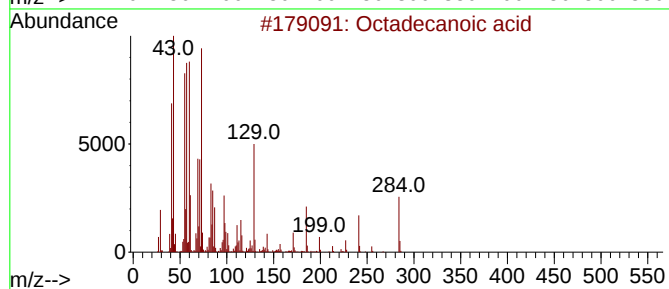
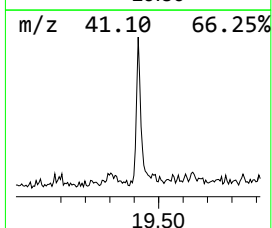
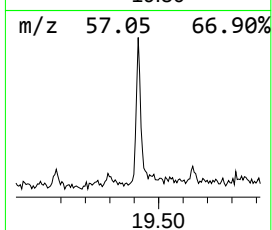
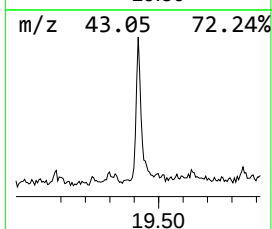
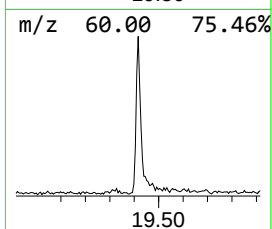
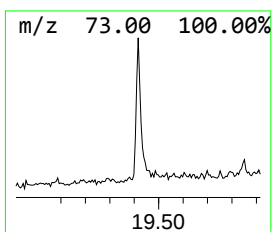
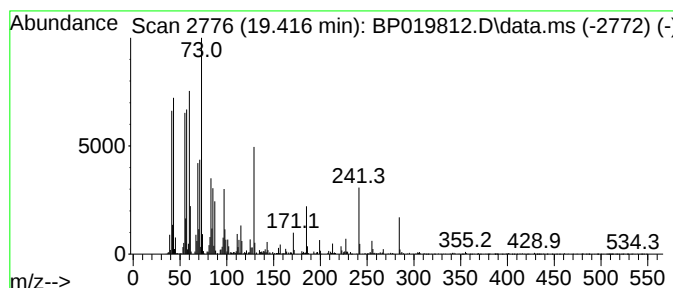
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	2.79 ng	192145	Chrysene-d12	21.375

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022124\
Data File : BP019812.D
Acq On : 21 Feb 2024 17:28
Operator : MA/JU
Sample : P1537-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

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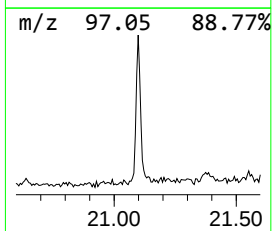
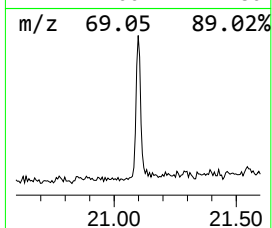
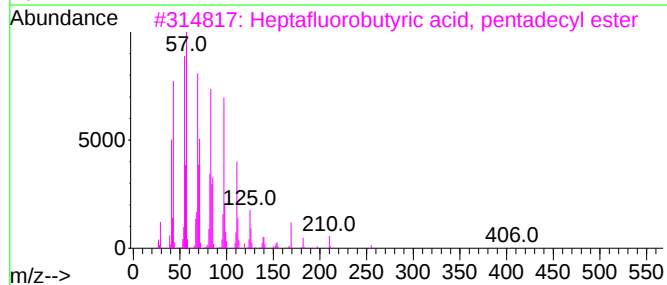
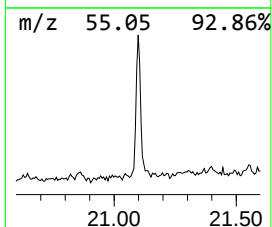
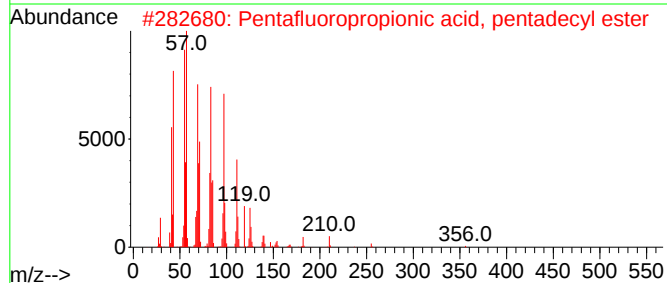
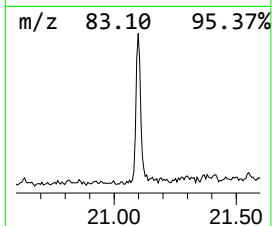
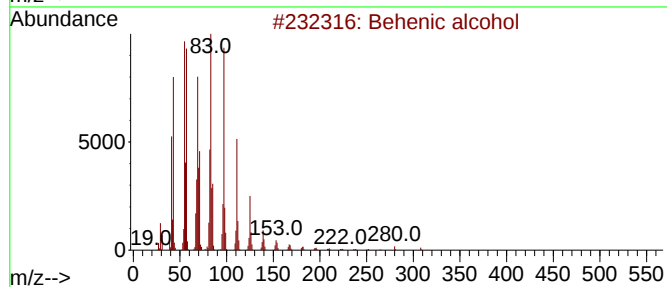
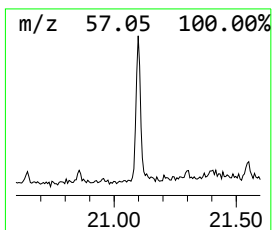
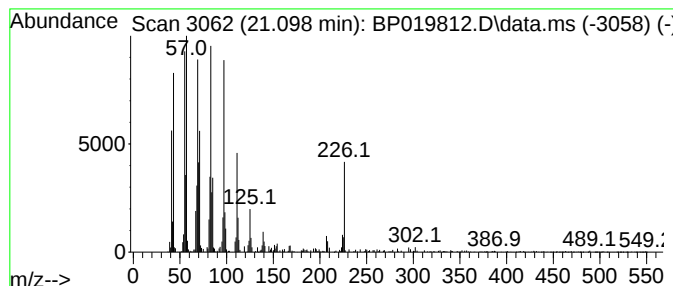
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	3.95 ng	272140	Chrysene-d12	21.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	93
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4			1-Tetracosene	336	C24H48	010192-32-2	93
5			1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022124\
Data File : BP019812.D
Acq On : 21 Feb 2024 17:28
Operator : MA/JU
Sample : P1537-04
Misc :
ALS Vial : 15 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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, ...	3.129	35.4	ng	739219	1	7.893	418234	20.0
Prenol	4.070	3.5	ng	73745	1	7.893	418234	20.0
4-Trifluoroacet...	4.305	3.5	ng	72199	1	7.893	418234	20.0
2-Pentanol, 4-m...	4.634	4.9	ng	101545	1	7.893	418234	20.0
1-Butanol, 3-me...	4.687	2.6	ng	54005	1	7.893	418234	20.0
2-Pentanone, 4-...	5.011	15.1	ng	315649	1	7.893	418234	20.0
unknown6.093	6.093	2.9	ng	61089	1	7.893	418234	20.0
unknown6.717	6.717	2.4	ng	49041	1	7.893	418234	20.0
n-Hexadecanoic ...	18.181	12.0	ng	595233	4	17.287	989808	20.0
Octadecanoic acid	19.416	2.8	ng	192145	5	21.375	1377080	20.0
Behenic alcohol	21.098	4.0	ng	272140	5	21.375	1377080	20.0