

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP013023\
 Data File : BP013662.D
 Acq On : 31 Jan 2023 00:53
 Operator : CG/JU
 Sample : 01329-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-7-BORING-2-14-21

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-BP012623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013662.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.217	3	5	10	rVB	1858665	1757449	16.27%	2.403%
2	3.258	10	12	22	rVB	95534	109789	1.02%	0.150%
3	5.211	337	344	358	rBV	1912742	2710279	25.09%	3.706%
4	5.675	416	423	438	rBV	4494422	6823705	63.18%	9.331%
5	7.293	687	698	713	rBV	4217623	6920888	64.08%	9.464%
6	8.146	835	843	849	rBV	759068	1221085	11.31%	1.670%
7	9.316	1034	1042	1055	rBV	2363378	3810618	35.28%	5.211%
8	10.975	1316	1324	1334	rBV	911927	1571293	14.55%	2.149%
9	13.404	1730	1737	1751	rBV	6315786	9179310	84.99%	12.552%
10	14.781	1964	1971	1983	rBV	1213860	1895961	17.56%	2.593%
11	16.134	2194	2201	2212	rBV	245949	380854	3.53%	0.521%
12	16.263	2216	2223	2244	rBV	4236036	6538050	60.54%	8.940%
13	17.533	2432	2439	2453	rBV	1431874	2113975	19.57%	2.891%
14	18.386	2579	2584	2595	rBV	574013	924724	8.56%	1.265%
15	19.492	2770	2772	2782	rVB5	63835	116862	1.08%	0.160%
16	19.610	2787	2792	2806	rBV	255455	459186	4.25%	0.628%
17	20.063	2863	2869	2881	rBV	8799051	10800105	100.00%	14.768%
18	21.280	3072	3076	3084	rBV	506417	724291	6.71%	0.990%
19	21.604	3127	3131	3137	rBV	1753228	2328137	21.56%	3.184%
20	21.727	3147	3152	3182	rBV	3694902	8455499	78.29%	11.562%
21	22.533	3286	3289	3299	rVB	420828	638554	5.91%	0.873%
22	22.921	3351	3355	3364	rVB	463865	699168	6.47%	0.956%
23	24.186	3563	3570	3580	rVB2	1320964	2949603	27.31%	4.033%

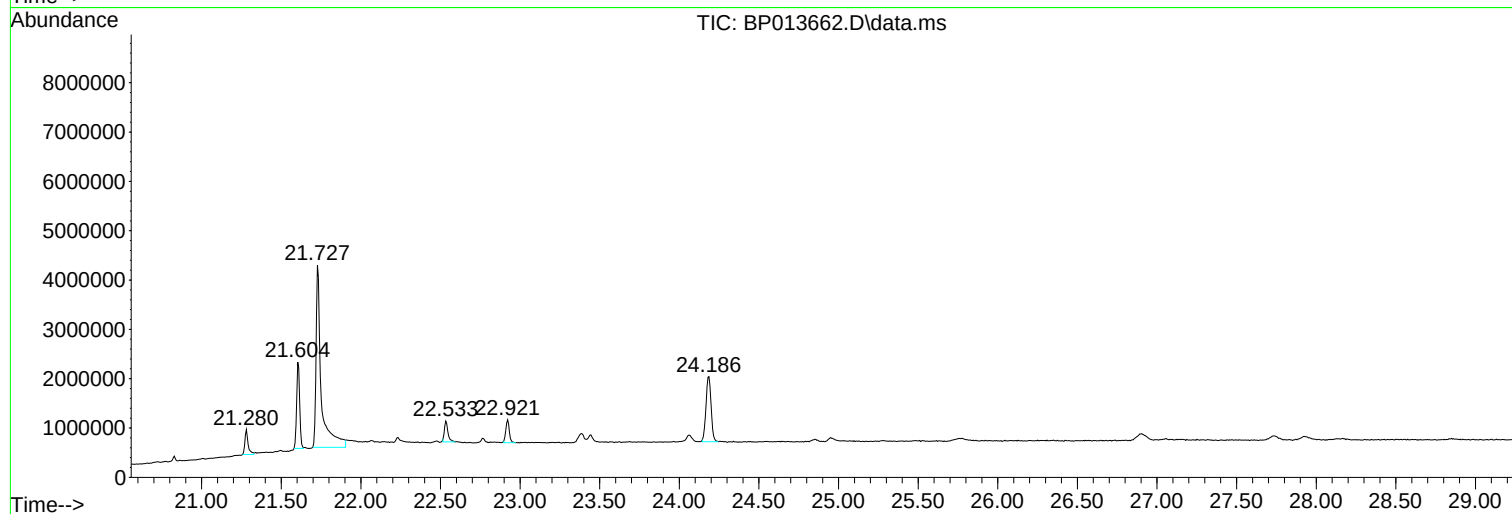
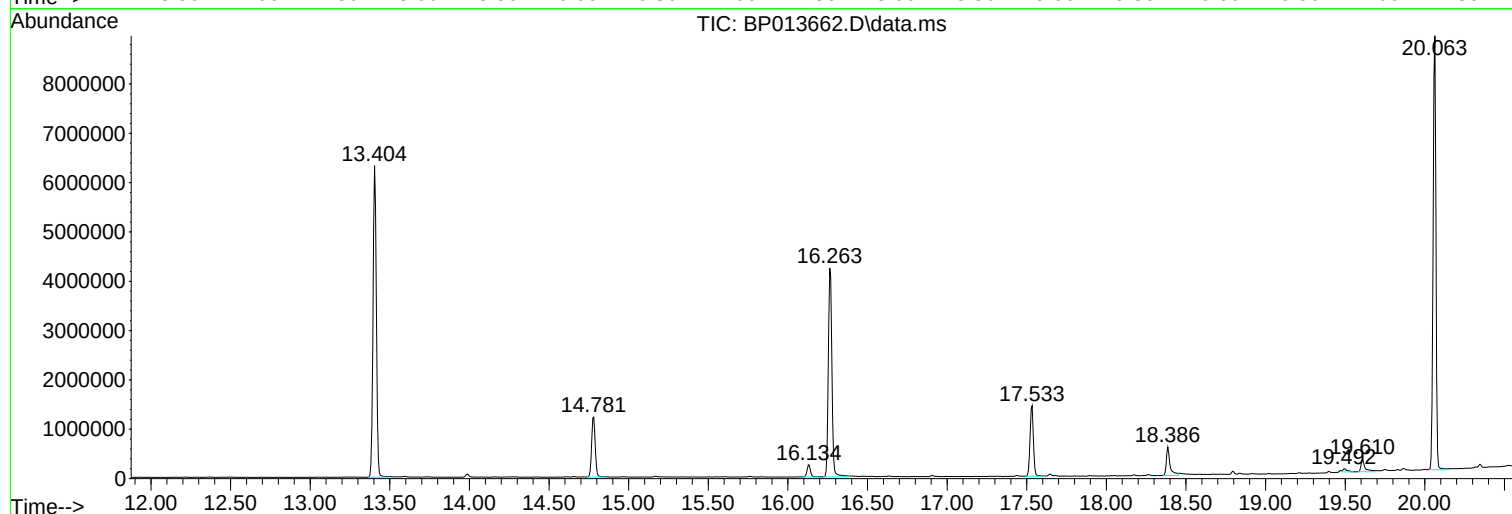
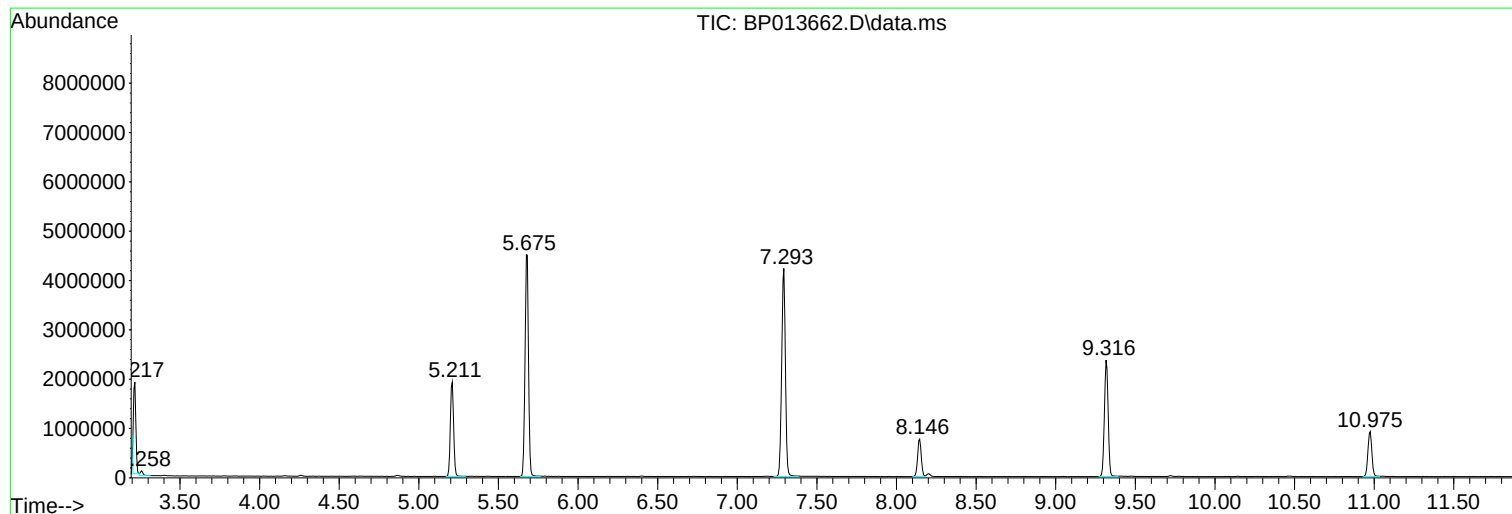
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Instrument :
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ClientSampleId :
COMP-7-BORING-2-14-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.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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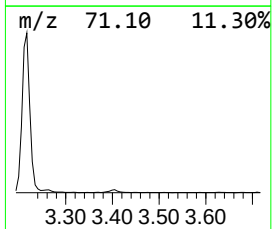
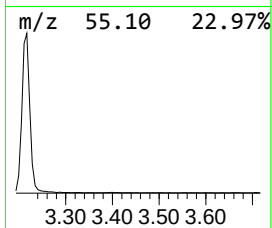
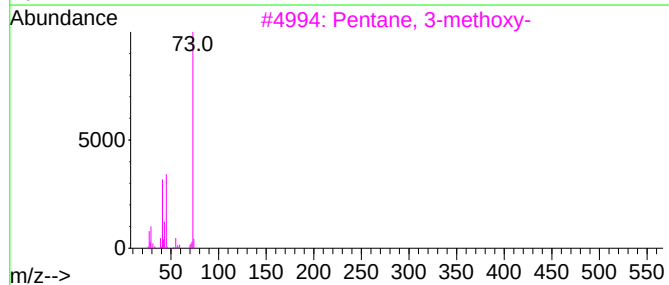
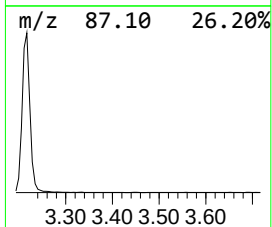
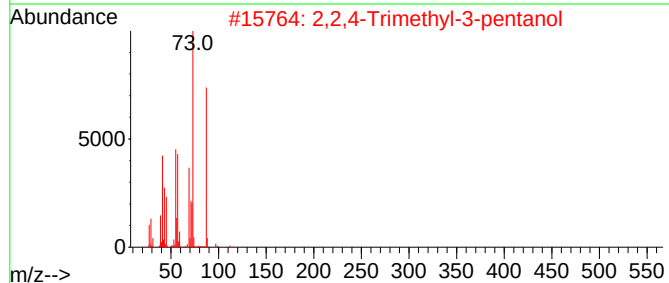
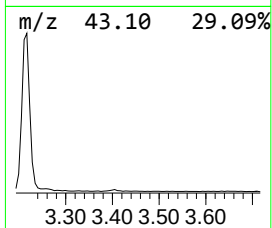
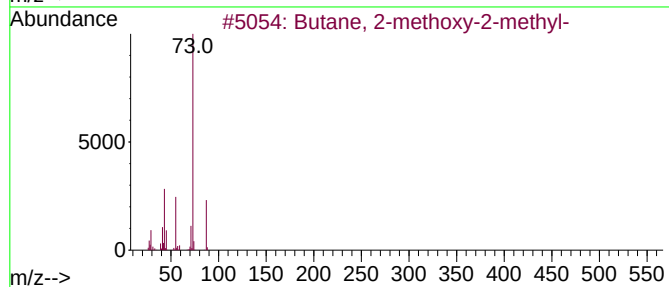
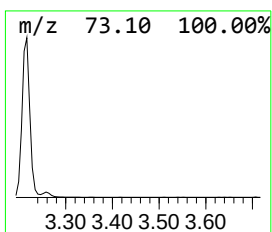
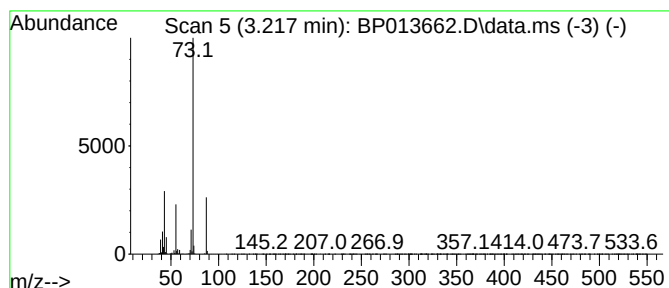
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.217	28.79 ng	1757450	1,4-Dichlorobenzene-d4	8.146

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	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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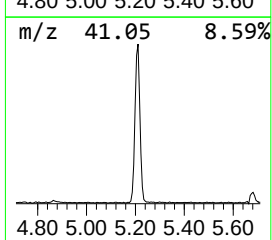
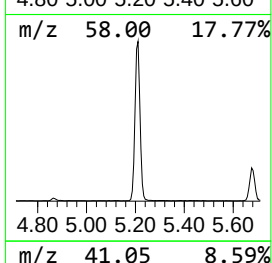
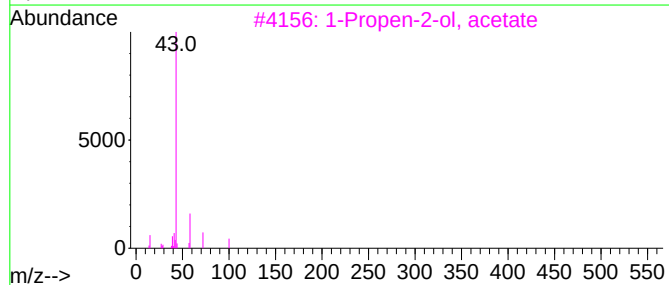
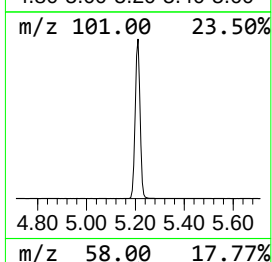
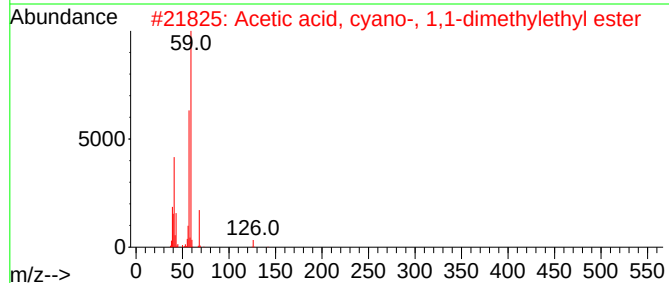
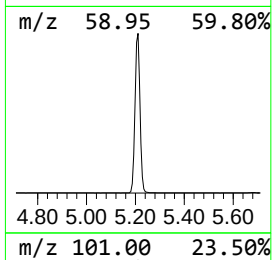
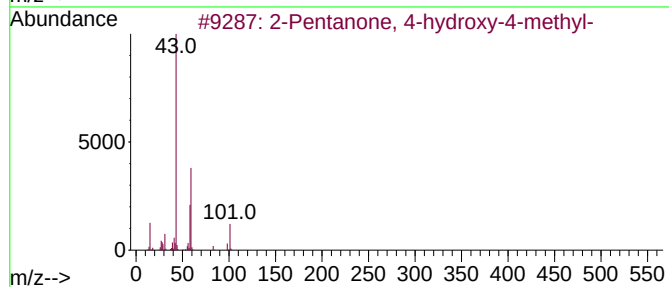
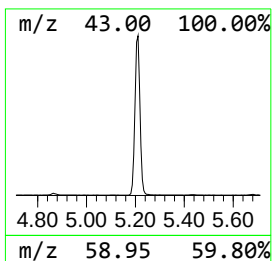
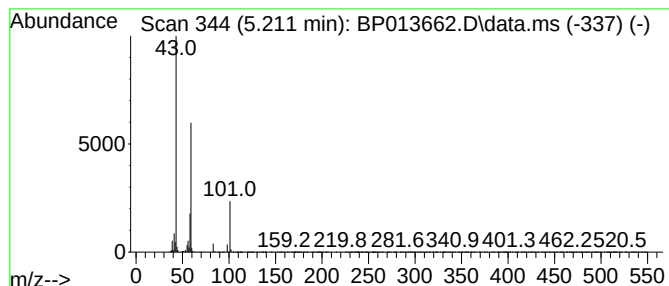
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.211	44.39 ng	2710280	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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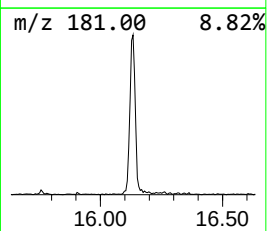
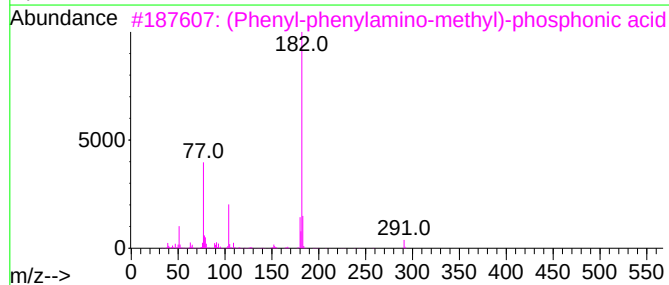
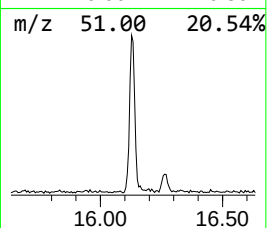
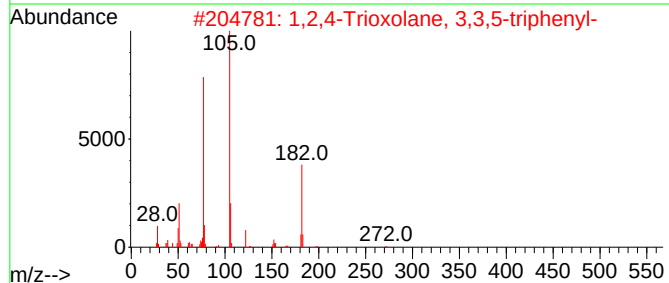
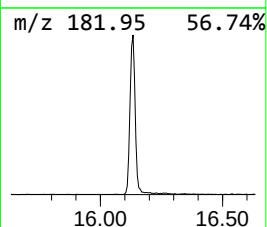
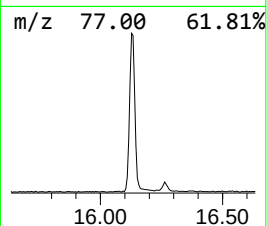
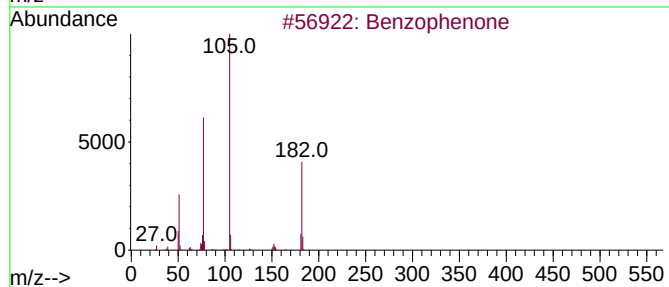
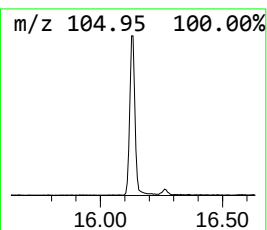
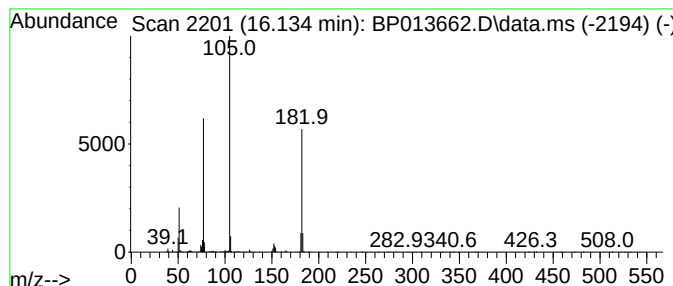
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.134	4.02 ng	380854	Acenaphthene-d10	14.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3			(Phenyl-phenylamino-methyl)-phos...	291	C15H18NO3P	026624-91-9	59
4			Benzoic acid, 2-benzoyl-	226	C14H10O3	000085-52-9	56
5			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	45



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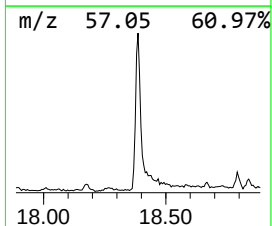
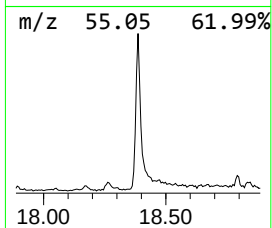
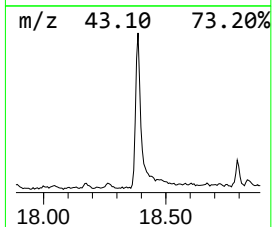
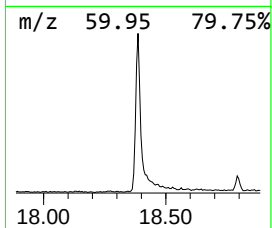
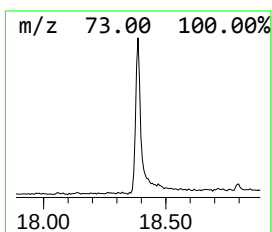
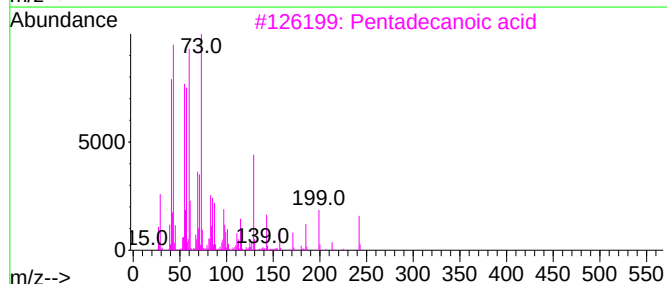
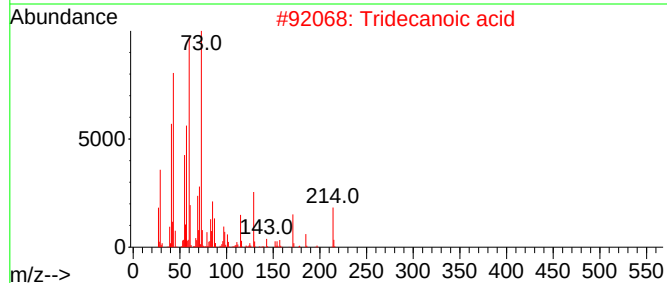
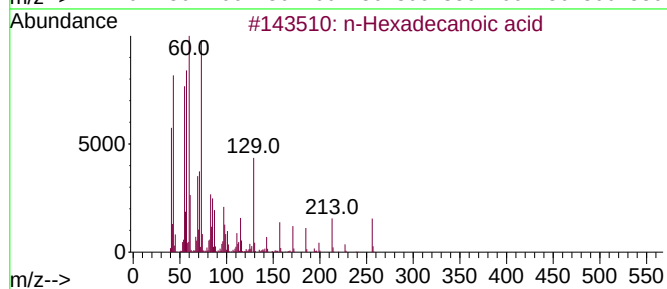
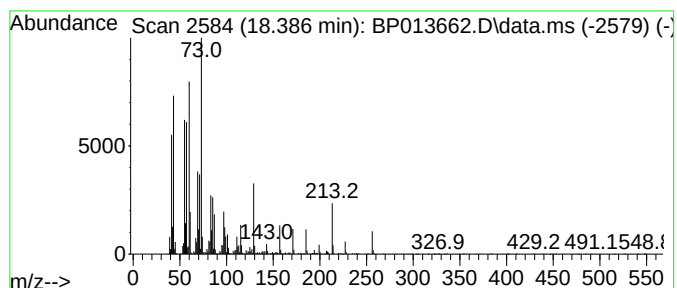
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.386	8.75 ng	924724	Phenanthrene-d10	17.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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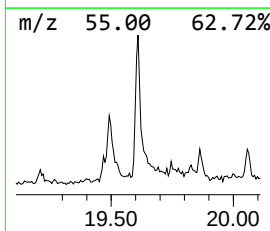
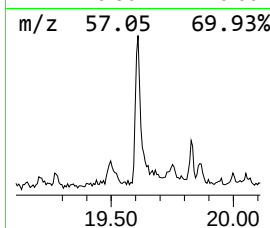
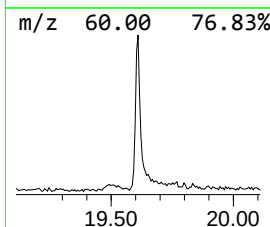
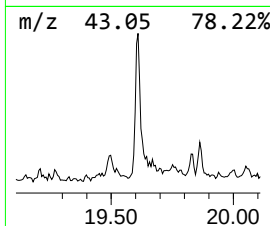
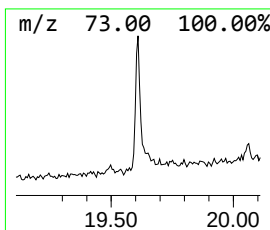
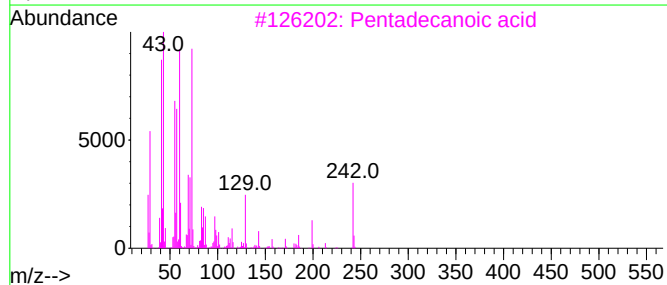
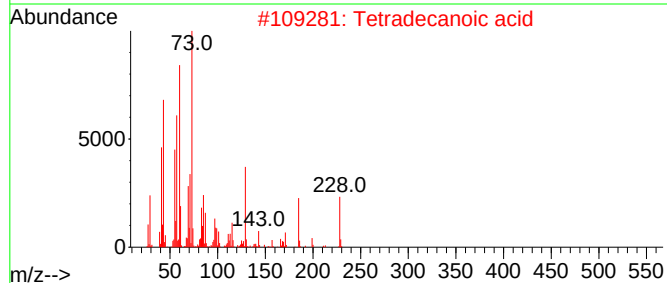
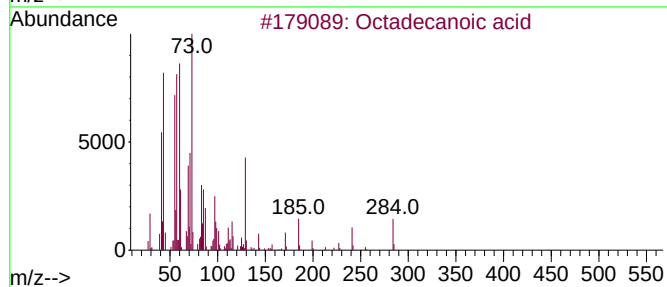
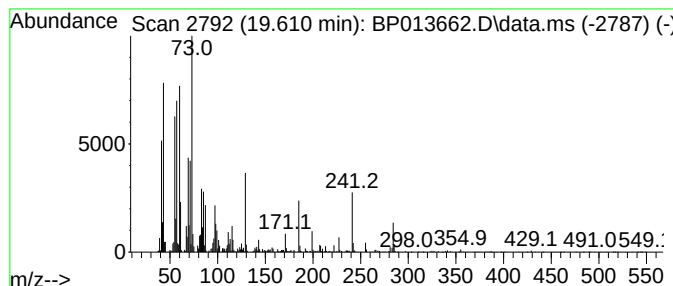
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.610	3.94 ng	459186	Chrysene-d12	21.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47



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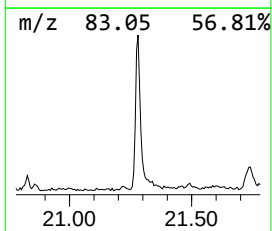
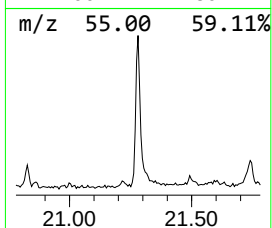
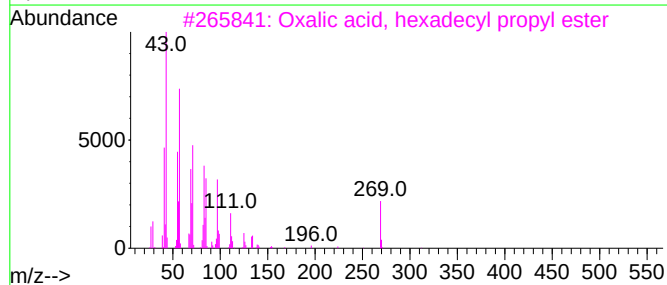
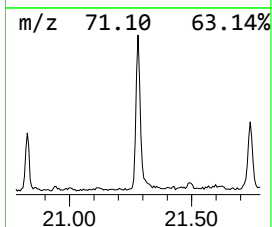
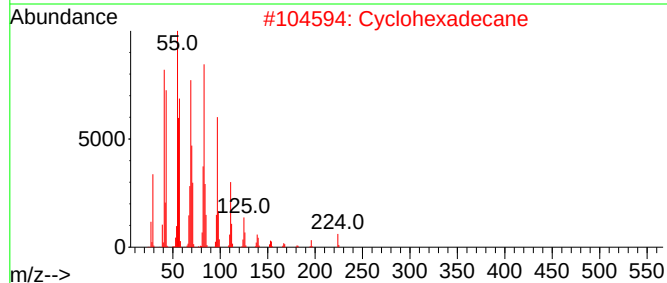
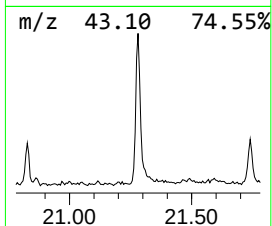
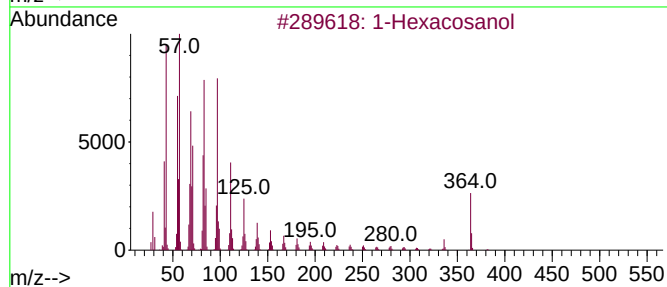
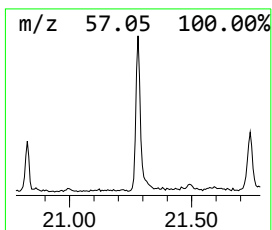
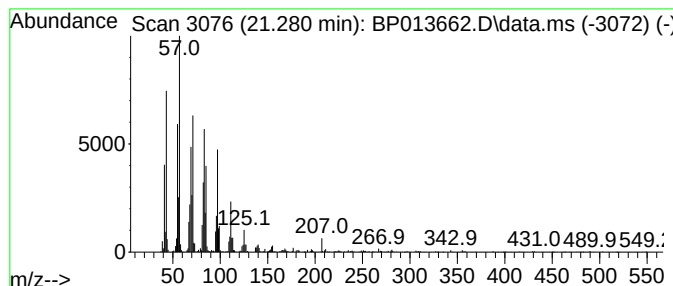
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.280	6.22 ng	724291	Chrysene-d12	21.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosanol	382	C26H54O	000506-52-5	91
2			Cyclohexadecane	224	C16H32	000295-65-8	91
3			Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	90
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	76
5			Cyclotriacontane	420	C30H60	000297-35-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP013023\
Data File : BP013662.D
Acq On : 31 Jan 2023 00:53
Operator : CG/JU
Sample : 01329-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-7-BORING-2-14-21

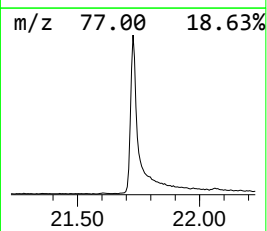
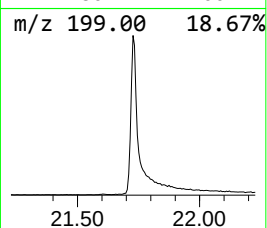
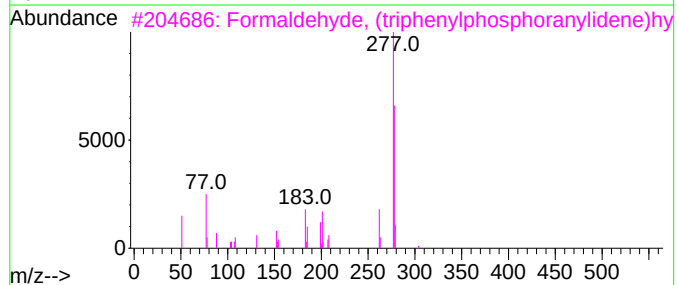
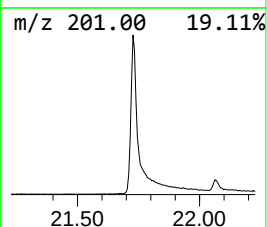
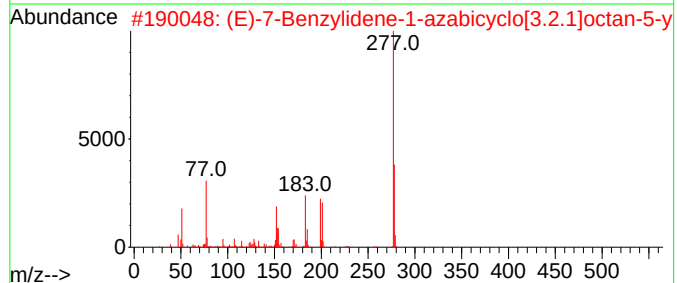
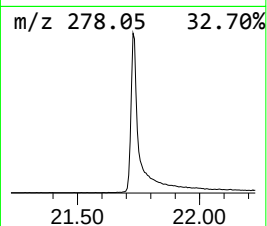
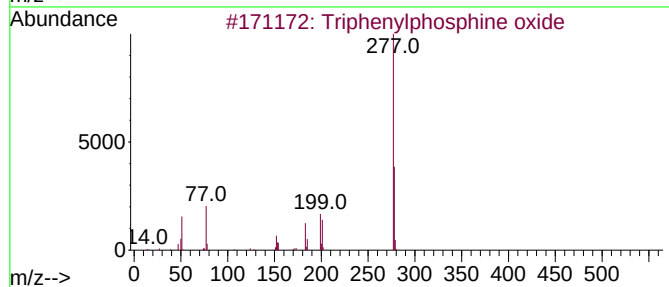
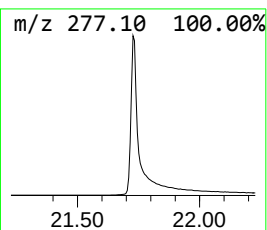
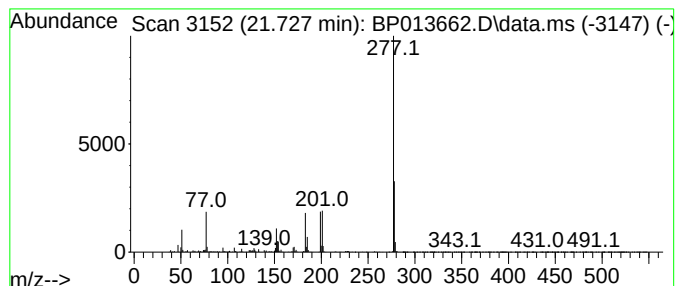
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.727	72.64 ng	8455500	Chrysene-d12	21.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3.1.0]hex-2-ene	293	C15H19N03S	1000483-83-4	87
3			Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	45
4			3-(3,4-Dichlorophenyl)-2-thioxo-1,2,3,4-tetrahydropyridine	277	C9H5Cl2NOS2	017046-34-3	37
5			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP013023\
Data File : BP013662.D
Acq On : 31 Jan 2023 00:53
Operator : CG/JU
Sample : 01329-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-7-BORING-2-14-21

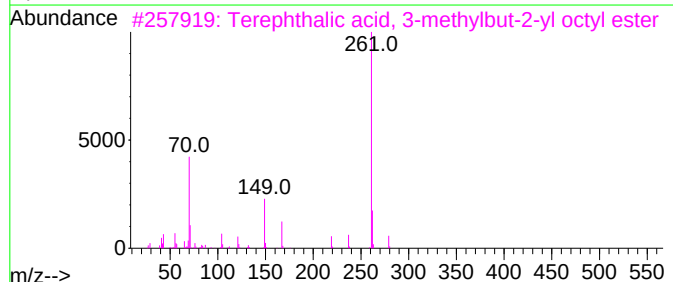
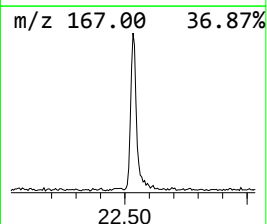
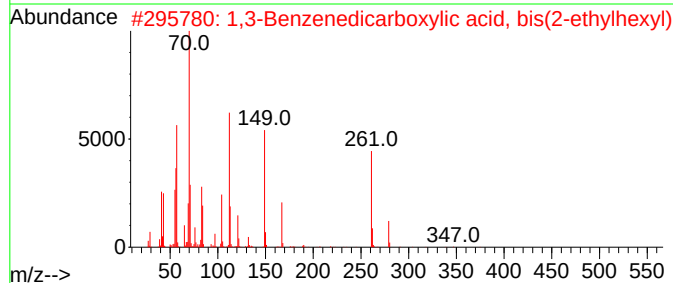
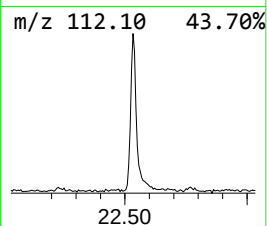
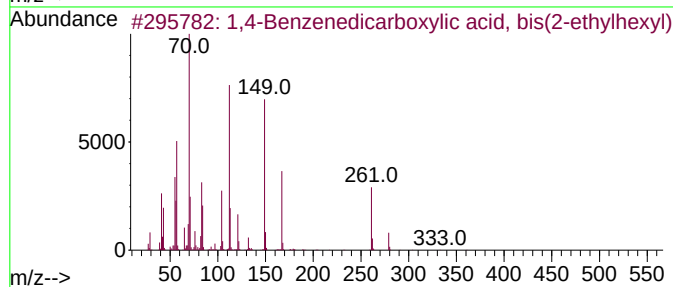
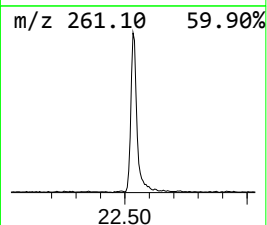
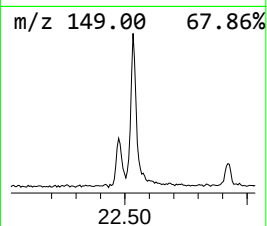
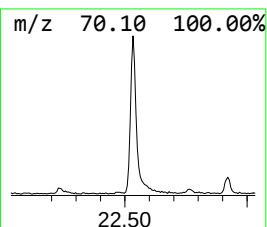
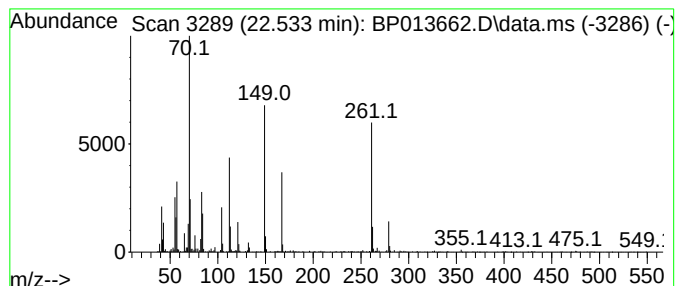
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,4-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.533	5.49 ng	638554	Chrysene-d12	21.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	52
4			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	50
5			Terephthalic acid, di(6-methylhe...	390	C24H38O4	1000416-00-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP013023\
Data File : BP013662.D
Acq On : 31 Jan 2023 00:53
Operator : CG/JU
Sample : 01329-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-7-BORING-2-14-21

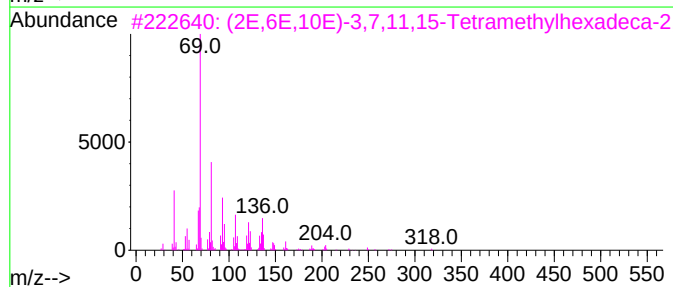
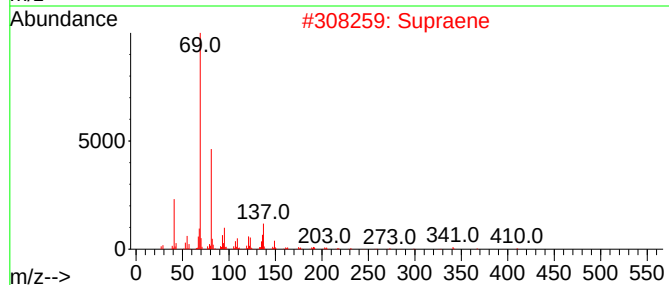
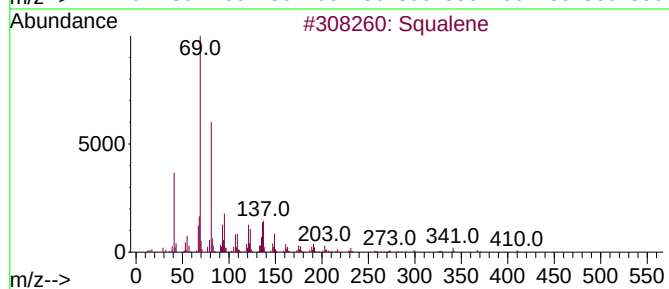
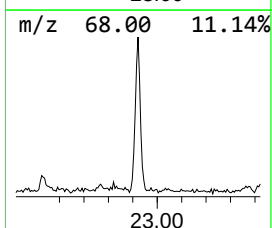
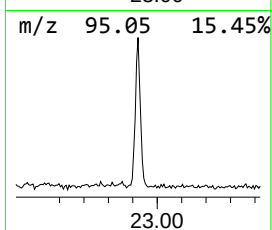
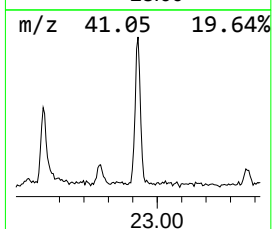
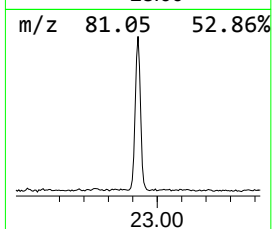
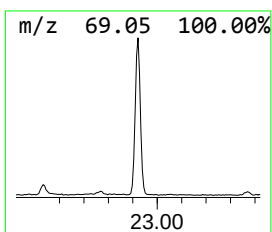
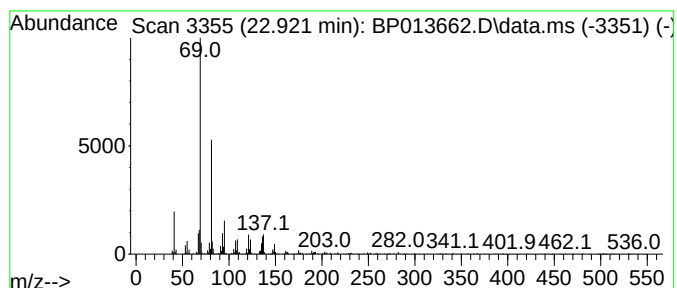
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.921	4.74 ng	699168	Perylene-d12	24.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	87
3			(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	83
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	80
5			trans-Farnesol	222	C15H26O	000106-28-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP013023\
Data File : BP013662.D
Acq On : 31 Jan 2023 00:53
Operator : CG/JU
Sample : 01329-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-7-BORING-2-14-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.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
Butane, 2-metho...	3.217	28.8	ng	1757450	1	8.146	1221090	20.0
2-Pentanone, 4-...	5.211	44.4	ng	2710280	1	8.146	1221090	20.0
Benzophenone	16.134	4.0	ng	380854	3	14.781	1895960	20.0
n-Hexadecanoic ...	18.386	8.8	ng	924724	4	17.534	2113980	20.0
Octadecanoic acid	19.610	3.9	ng	459186	5	21.604	2328140	20.0
1-Hexacosanol	21.280	6.2	ng	724291	5	21.604	2328140	20.0
Triphenylphosph...	21.727	72.6	ng	8455500	5	21.604	2328140	20.0
1,4-Benzenedica...	22.533	5.5	ng	638554	5	21.604	2328140	20.0
Squalene	22.921	4.7	ng	699168	6	24.186	2949600	20.0