

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
 Data File : BP008279.D
 Acq On : 08 Dec 2021 14:27
 Operator : CG/JU
 Sample : M4953-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A3718

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-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008279.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	398	405	415	rBV	770326	1122167	18.20%	4.021%
2	6.964	665	676	689	rBV	429353	786092	12.75%	2.816%
3	7.775	805	814	822	rBV	325423	533725	8.66%	1.912%
4	8.940	1004	1012	1023	rBV	1195748	2040272	33.09%	7.310%
5	9.363	1075	1084	1090	rBV	46796	75116	1.22%	0.269%
6	10.375	1248	1256	1266	rBV	66740	153182	2.48%	0.549%
7	10.569	1282	1289	1297	rBV	424317	715416	11.60%	2.563%
8	12.269	1572	1578	1587	rBV2	35506	90801	1.47%	0.325%
9	13.046	1702	1710	1722	rBV	3248557	4777374	77.48%	17.117%
10	14.087	1881	1887	1903	rVB2	79127	146370	2.37%	0.524%
11	14.428	1938	1945	1952	rBV	687086	1024944	16.62%	3.672%
12	15.257	2077	2086	2090	rBV2	115625	259640	4.21%	0.930%
13	15.804	2171	2179	2184	rBV4	34910	83718	1.36%	0.300%
14	15.928	2193	2200	2208	rBV	2121786	3120421	50.61%	11.180%
15	17.122	2397	2403	2408	rVB	109843	142475	2.31%	0.510%
16	17.192	2408	2415	2422	rBV	842462	1207682	19.59%	4.327%
17	17.492	2461	2466	2475	rBV4	47061	103205	1.67%	0.370%
18	17.622	2479	2488	2493	rVV4	27171	72656	1.18%	0.260%
19	18.098	2564	2569	2574	rBV	175656	260064	4.22%	0.932%
20	18.157	2576	2579	2583	rVB	64993	83044	1.35%	0.298%
21	18.504	2634	2638	2643	rVB	94861	110797	1.80%	0.397%
22	18.910	2704	2707	2715	rBV2	44523	77055	1.25%	0.276%
23	19.216	2756	2759	2766	rVB2	48658	78881	1.28%	0.283%
24	19.333	2775	2779	2786	rBV3	62601	93797	1.52%	0.336%
25	19.575	2817	2820	2829	rVB	38667	75838	1.23%	0.272%
26	19.769	2847	2853	2866	rVB	5158078	6166040	100.00%	22.092%
27	20.445	2964	2968	2975	rBV	198651	241346	3.91%	0.865%
28	20.516	2977	2980	2984	rVV	117743	122396	1.99%	0.439%
29	20.975	3053	3058	3061	rBV	89223	146072	2.37%	0.523%
30	21.016	3061	3065	3072	rVV2	334266	531705	8.62%	1.905%
31	21.075	3072	3075	3081	rVV	125748	168965	2.74%	0.605%
32	21.210	3095	3098	3105	rBV	229030	265679	4.31%	0.952%
33	21.298	3107	3113	3117	rVV2	893867	1305404	21.17%	4.677%
34	21.339	3117	3120	3129	rVB	179595	265612	4.31%	0.952%
35	22.133	3252	3255	3261	rVB	116306	146879	2.38%	0.526%
36	22.545	3321	3325	3329	rBV	219652	293759	4.76%	1.052%

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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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37 23.692 3514 3520 3530 rVB2 496330 1022324 16.58% 3.663%

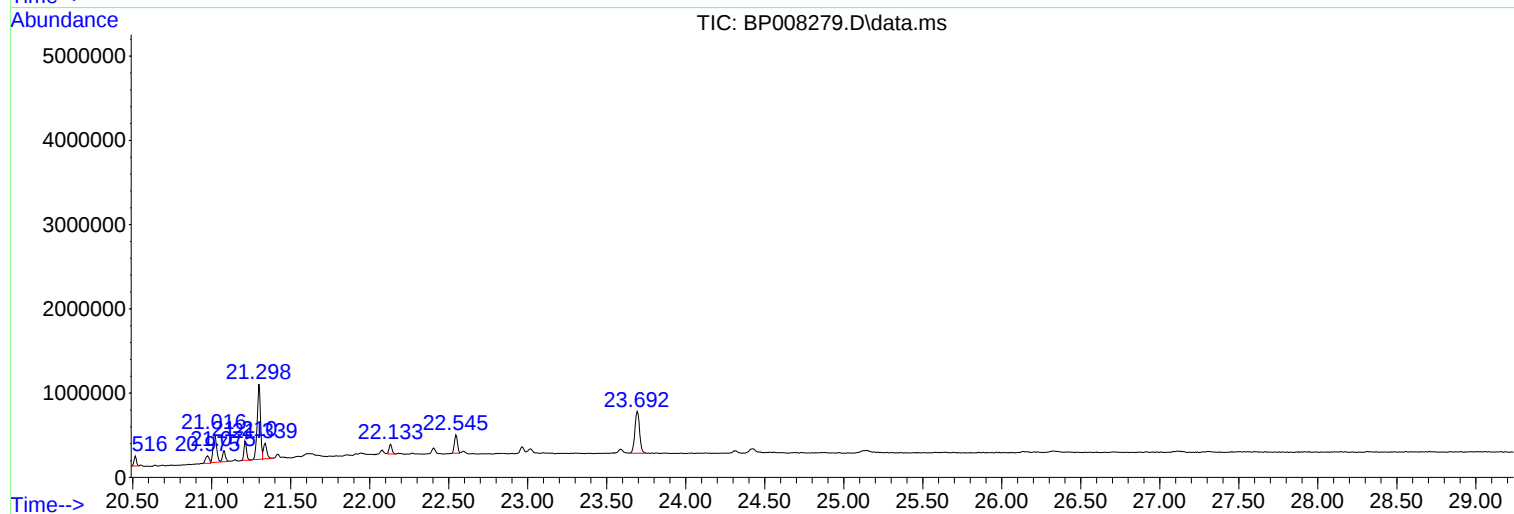
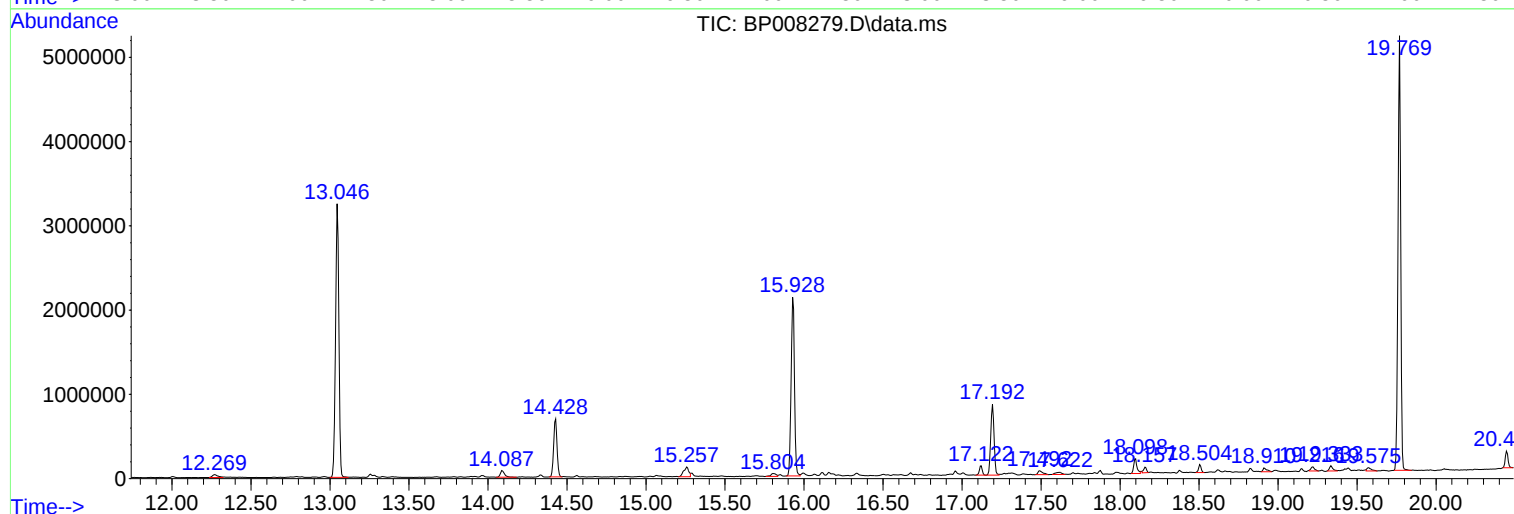
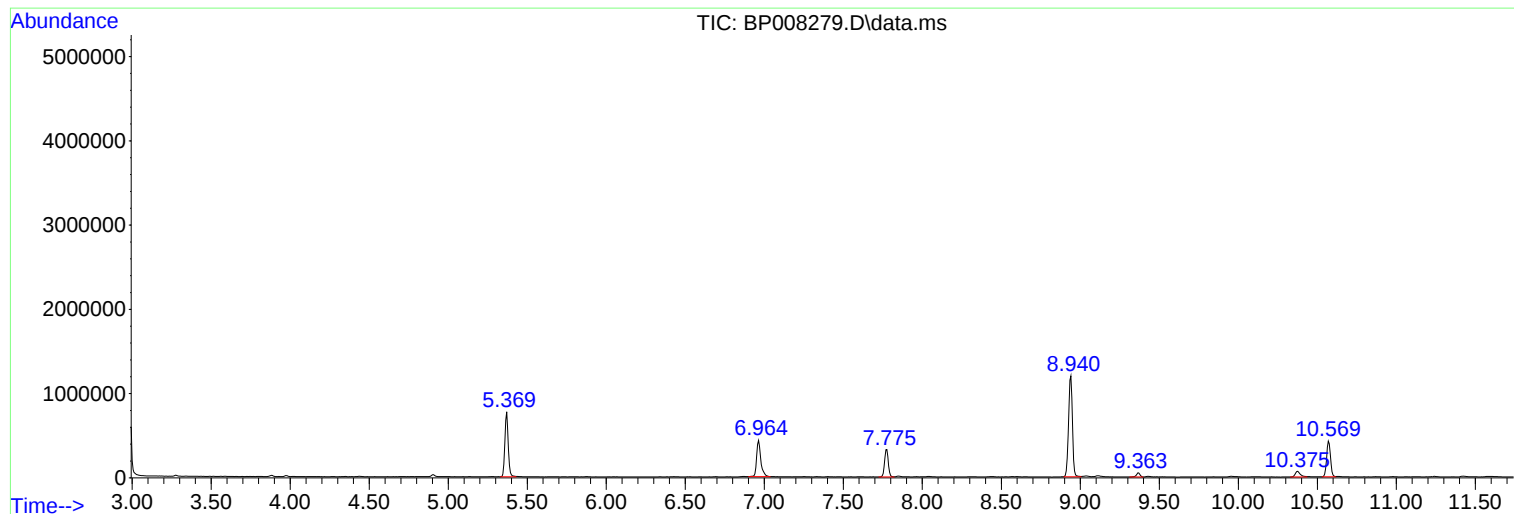
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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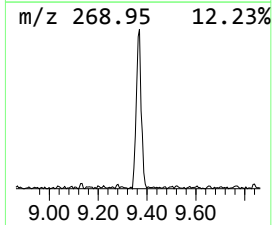
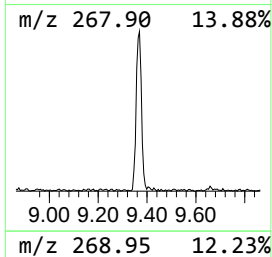
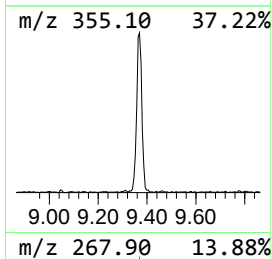
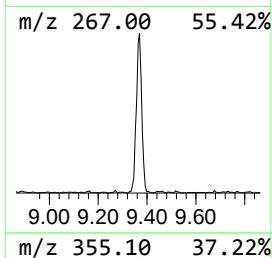
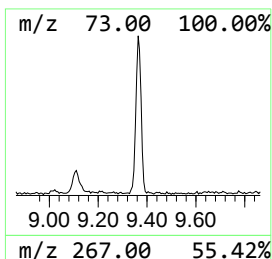
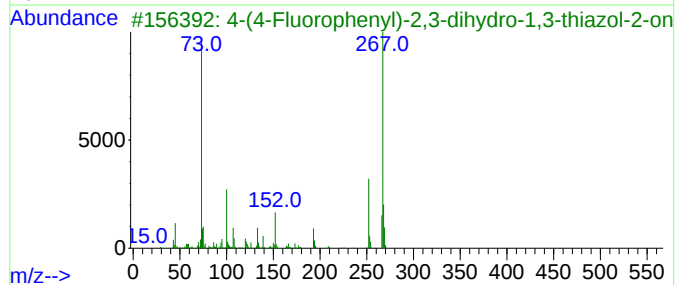
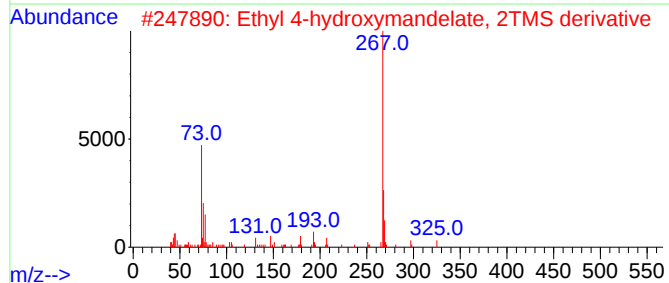
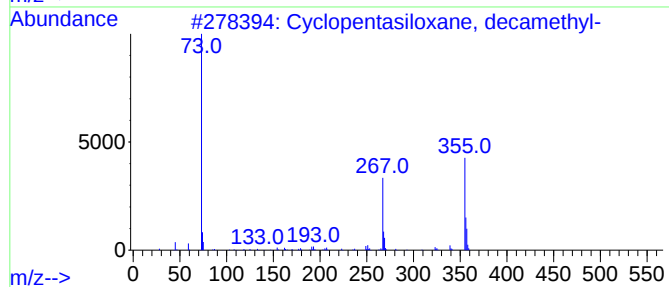
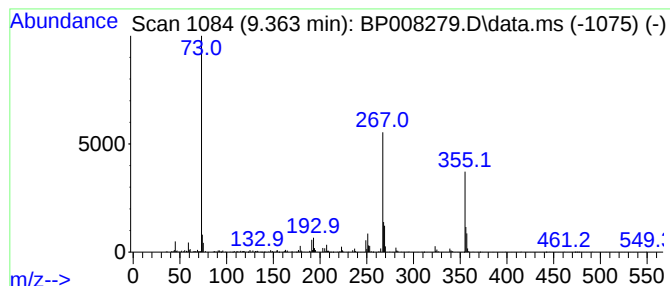
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentasiloxane, decamet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.363	2.10 ng	75116	Naphthalene-d8	10.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	59
2			Ethyl 4-hydroxymandelate, 2TMS d...	340	C16H28O4Si2	1010071-53-3	40
3			4-(4-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FNOSi	1010501-61-0	38
4			2-[(3-Chloro-2-methylphenyl)amin...	357	C15H28ClN3OSi2	1000514-51-8	38
5			4-(2-Acetylamino-1-(trimethylsil...	339	C16H29NO3Si2	1000373-43-5	38



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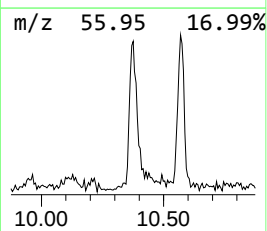
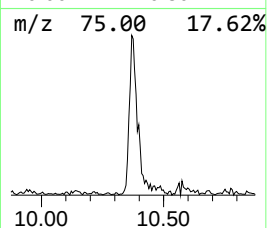
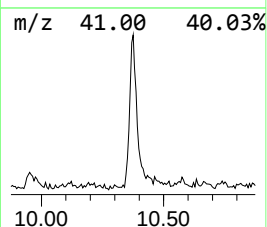
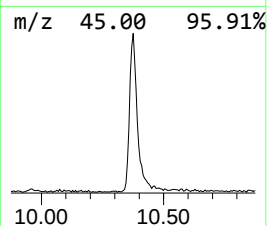
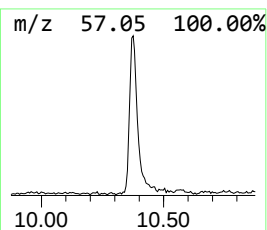
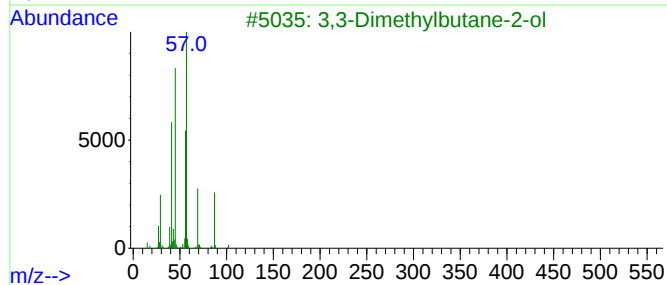
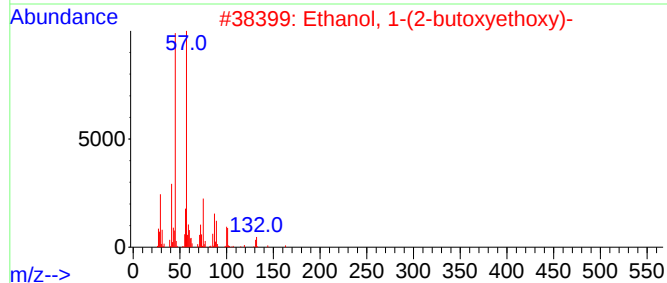
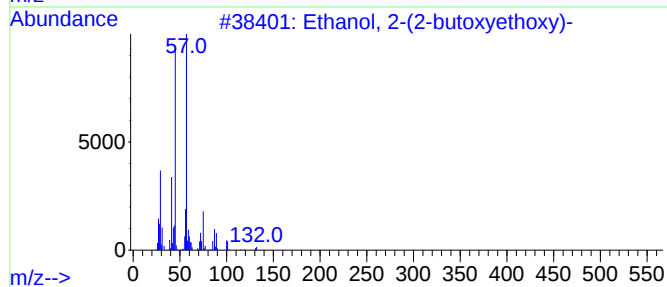
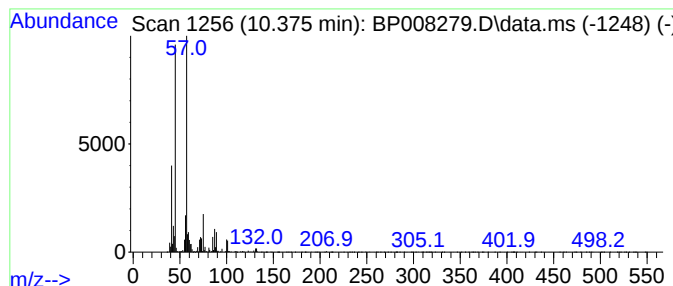
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.375	4.28 ng	153182	Naphthalene-d8	10.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50
5			Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	50



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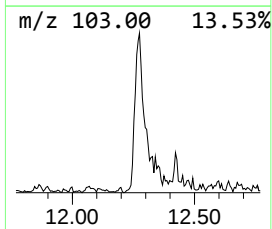
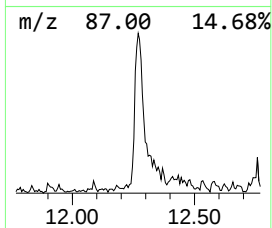
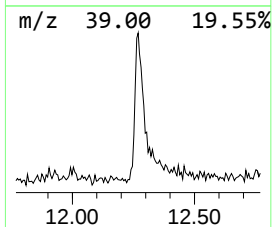
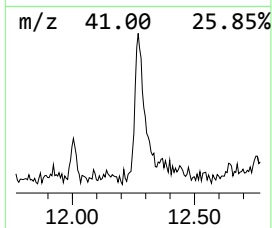
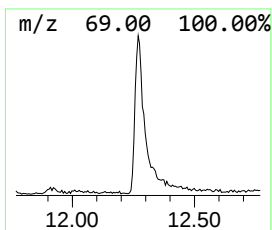
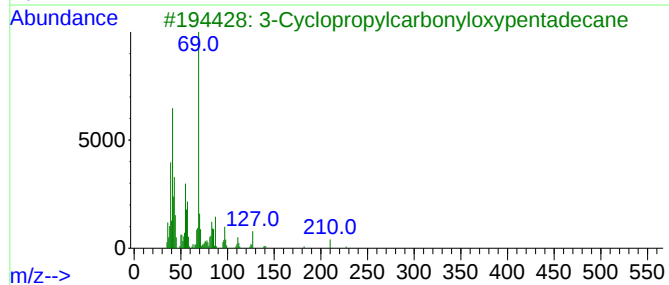
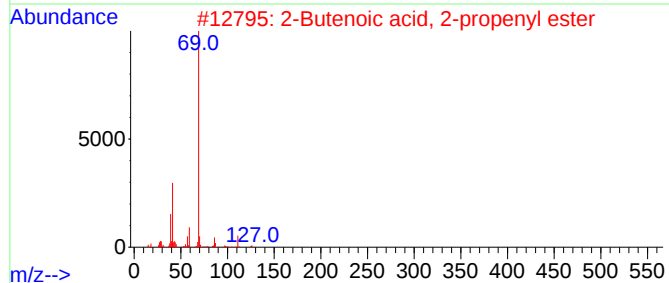
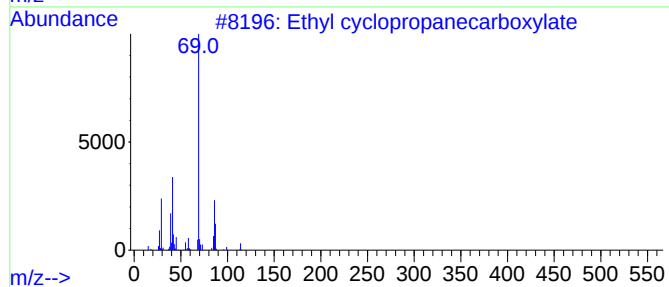
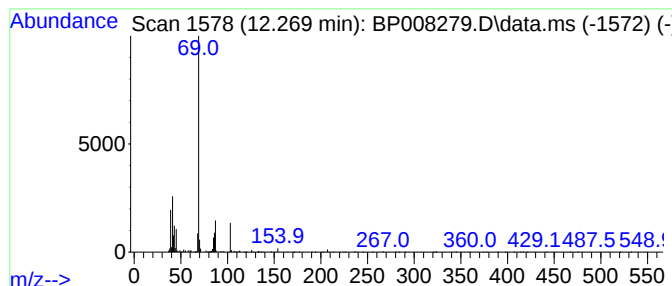
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethyl cyclopropanecarboxylate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.269	2.54 ng	90801	Naphthalene-d8	10.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	50
2			2-Butenoic acid, 2-propenyl ester	126	C7H10O2	020474-93-5	42
3			3-Cyclopropylcarbonyloxypentadecane	296	C19H36O2	1000245-59-0	36
4			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	33
5			2,4-Dinitrophenyl crotonate	252	C10H8N2O6	069817-88-5	28



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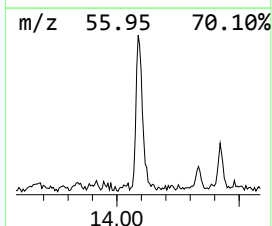
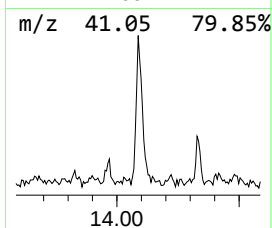
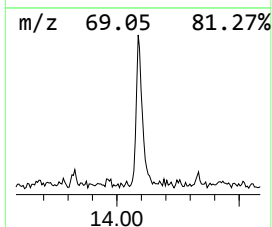
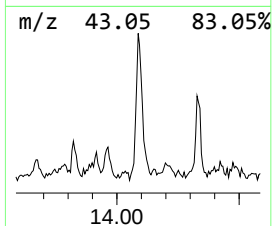
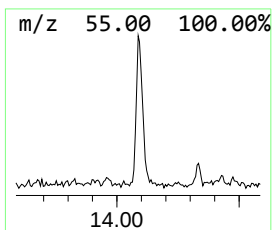
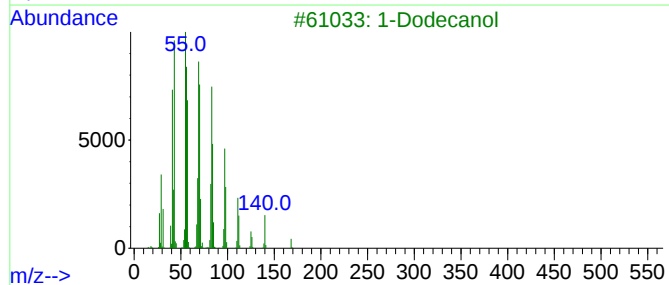
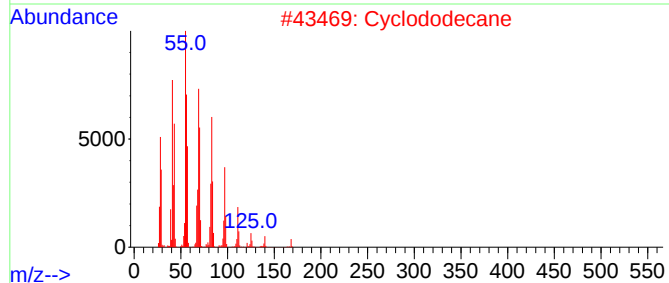
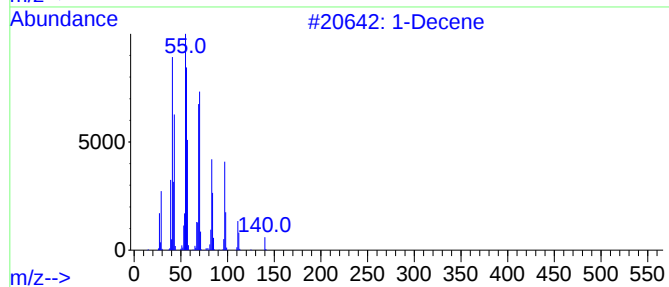
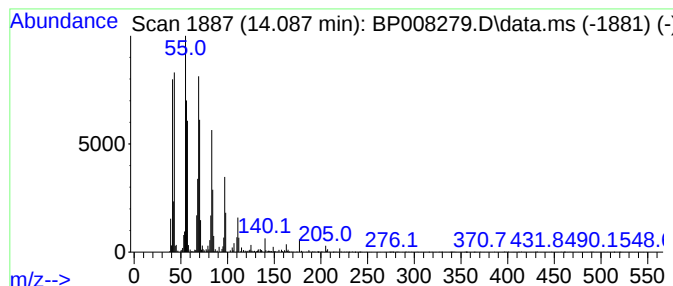
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Peak Number 4 1-Decene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.087	2.86 ng	146370	Acenaphthene-d10	14.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Decene	140	C10H20	000872-05-9	91
2		Cyclododecane	168	C12H24	000294-62-2	91
3		1-Dodecanol	186	C12H26O	000112-53-8	91
4		Cyclopropane, nonyl-	168	C12H24	074663-85-7	90
5		7-Tetradecene, (E)-	196	C14H28	041446-63-3	87



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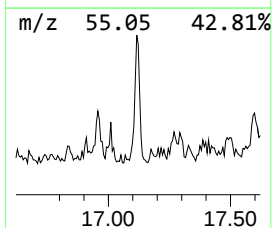
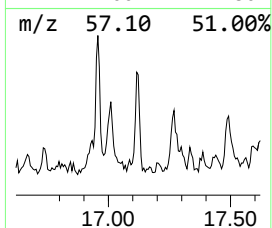
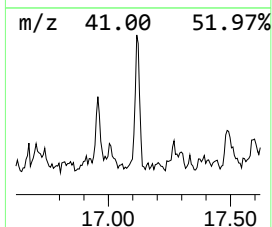
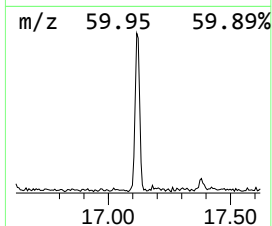
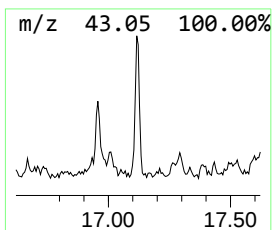
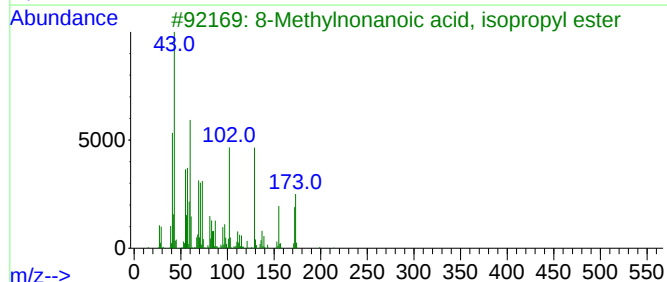
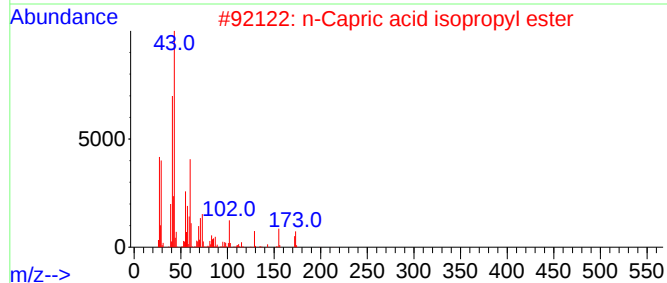
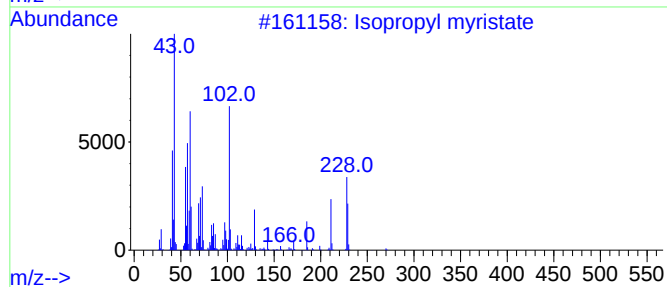
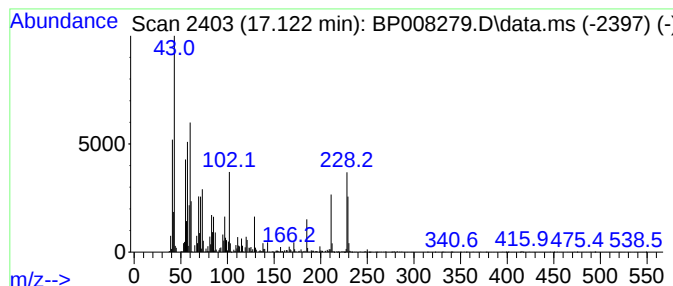
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.122	2.36 ng	142475	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl myristate	270	C17H34O2	000110-27-0	87
2			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	49
3			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	43
4			Docosanoic acid, isopropyl ester	382	C25H50O2	1000405-13-7	22
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008279.D
Acq On : 08 Dec 2021 14:27
Operator : CG/JU
Sample : M4953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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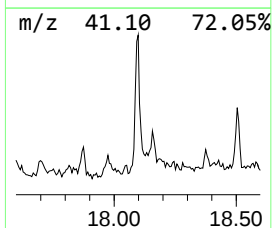
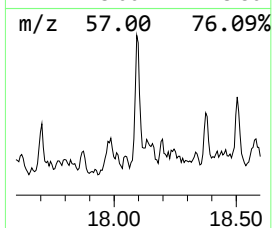
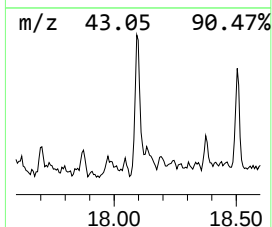
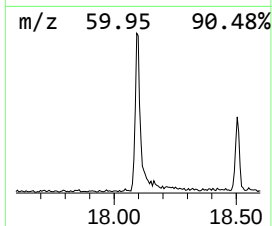
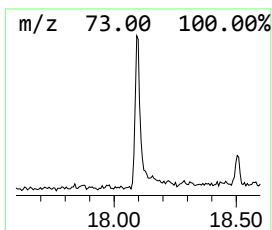
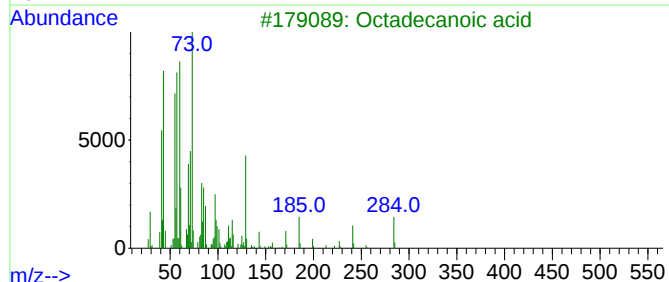
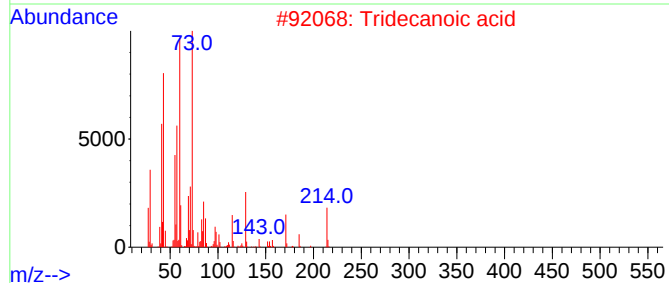
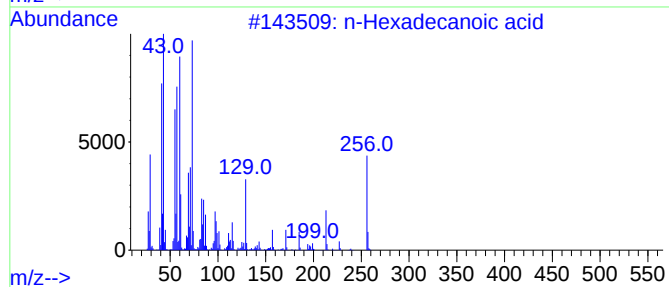
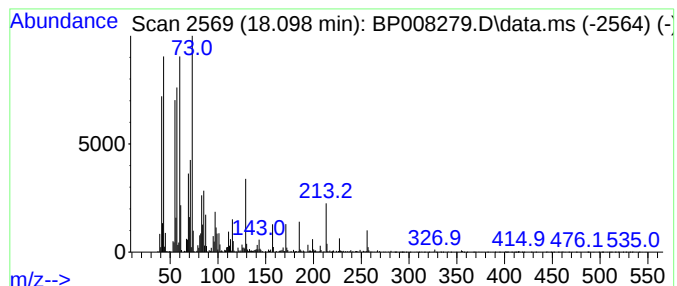
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	4.31 ng	260064	Phenanthrene-d10	17.192

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Octadecanoic acid	284	C18H36O2	000057-11-4	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008279.D
Acq On : 08 Dec 2021 14:27
Operator : CG/JU
Sample : M4953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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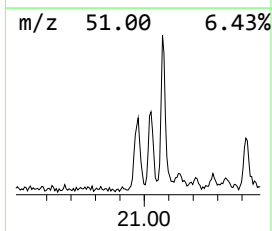
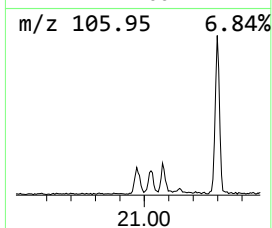
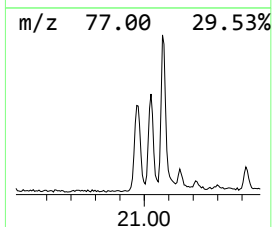
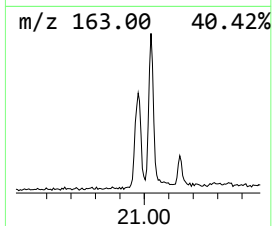
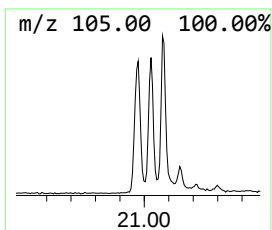
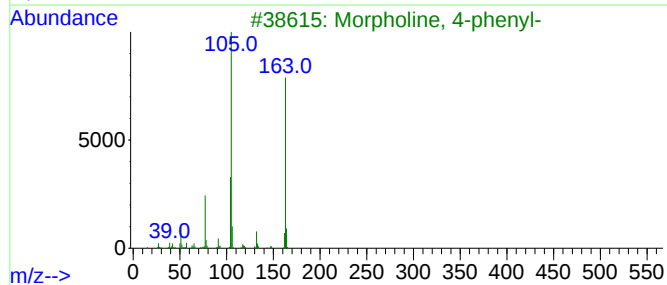
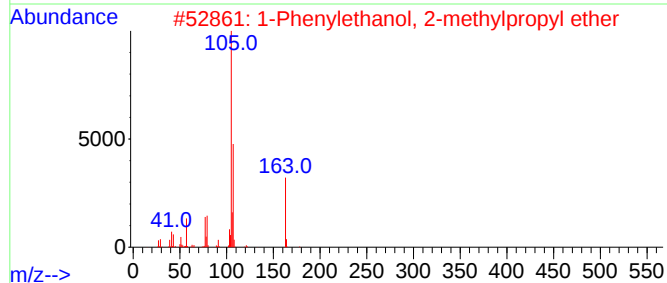
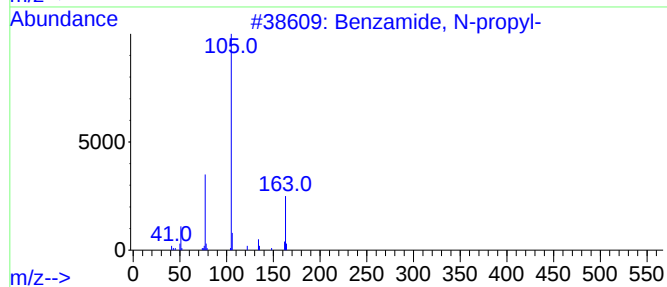
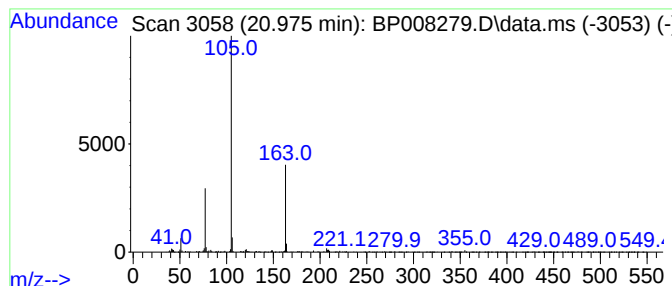
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown20.974 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	2.24 ng	146072	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	45
2			1-Phenylethanol, 2-methylpropyl ...	178	C12H18O	1000394-69-1	42
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	40
4			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	40
5			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008279.D
Acq On : 08 Dec 2021 14:27
Operator : CG/JU
Sample : M4953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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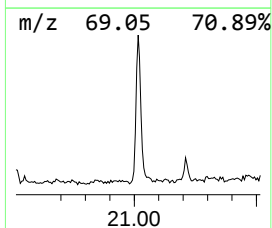
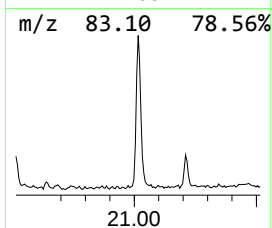
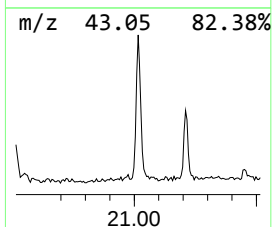
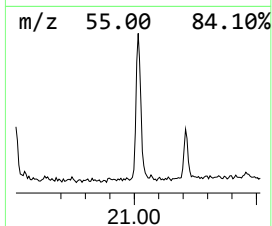
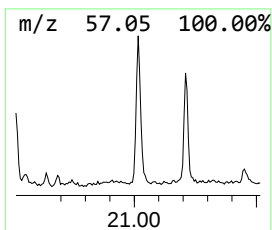
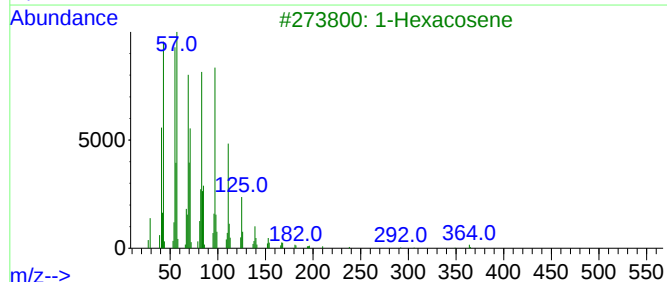
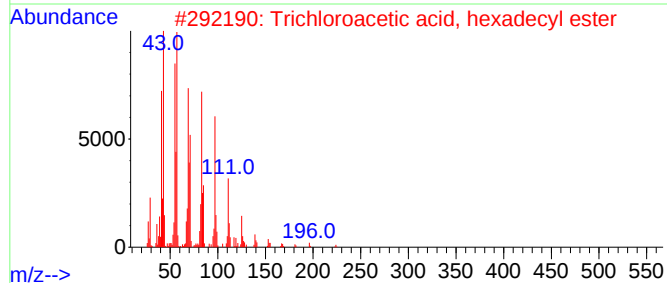
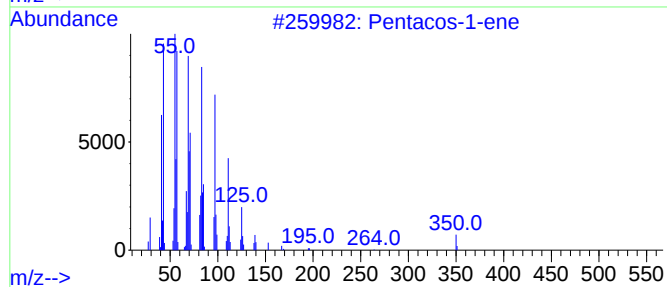
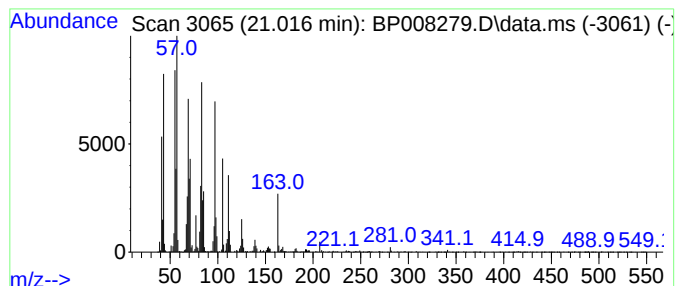
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacos-1-ene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.016	8.15 ng	531705	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacos-1-ene	350	C25H50	016980-85-1	93
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3			1-Hexacosene	364	C26H52	018835-33-1	93
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008279.D
Acq On : 08 Dec 2021 14:27
Operator : CG/JU
Sample : M4953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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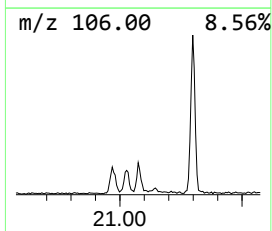
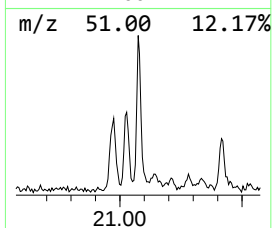
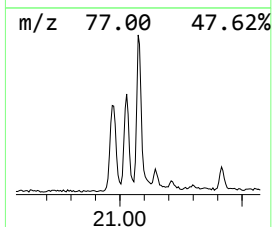
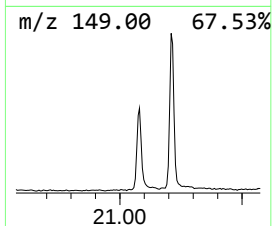
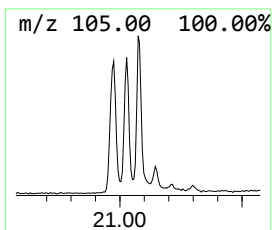
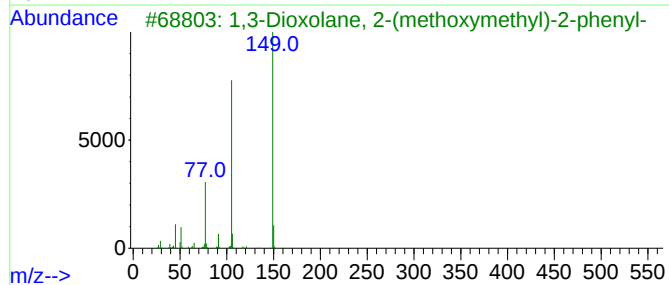
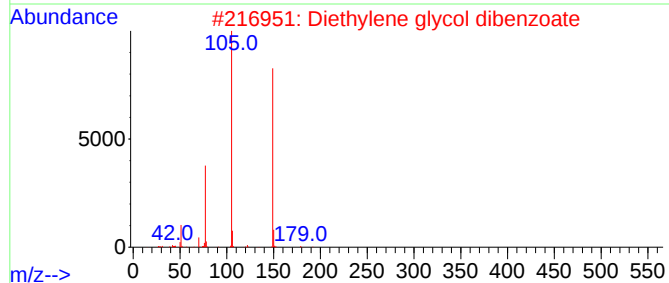
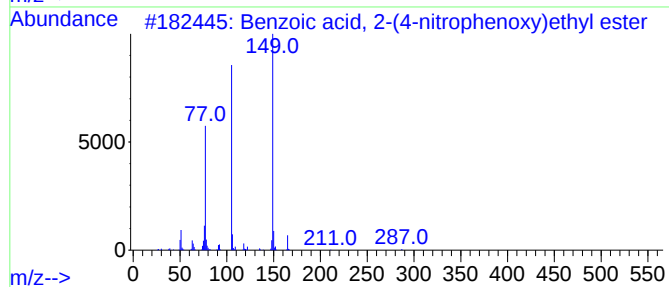
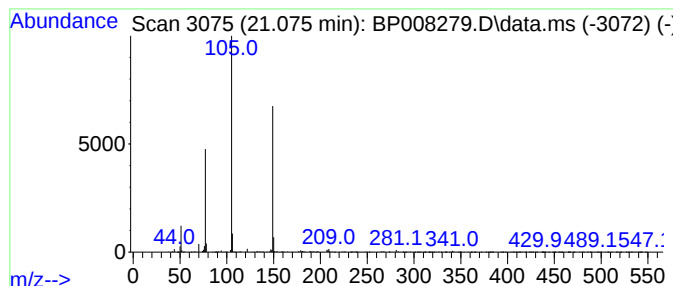
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzoic acid, 2-(4-nitrophe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.075	2.59 ng	168965	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
4			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
5			7-Methoxy-2-phenyl-1,3-benzoxazo...	250	C15H10N2O2	1000436-00-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008279.D
Acq On : 08 Dec 2021 14:27
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Sample : M4953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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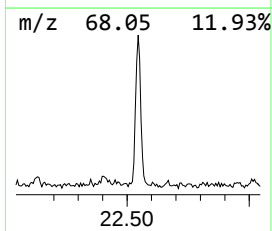
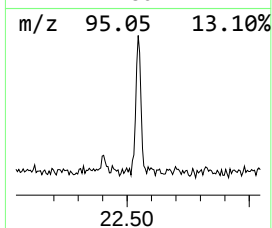
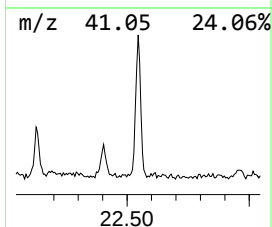
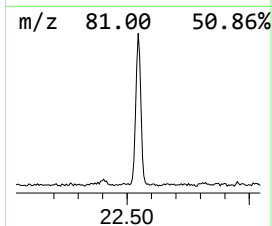
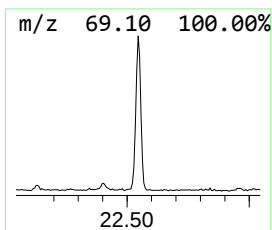
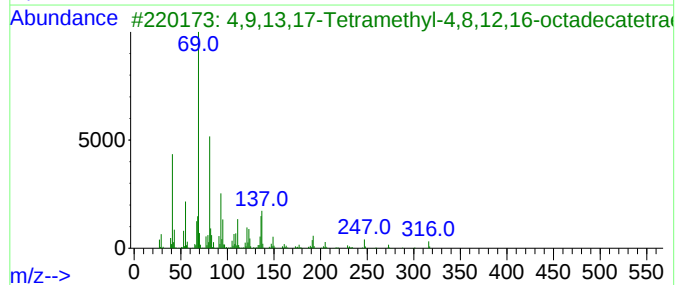
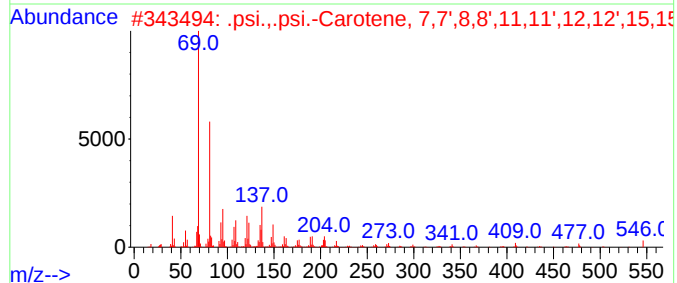
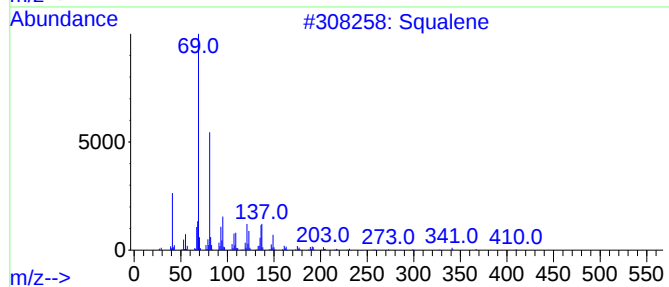
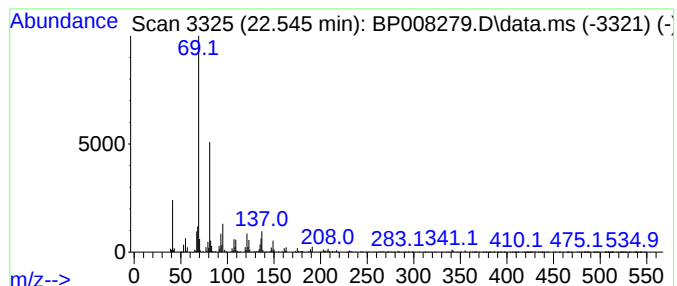
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.545	5.75 ng	293759	Perylene-d12	23.692

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Squalene	410	C30H50	000111-02-4	92
2		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H360	056882-09-8	72
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H280	066408-55-7	64
5		trans-Farnesol	222	C15H260	000106-28-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008279.D
Acq On : 08 Dec 2021 14:27
Operator : CG/JU
Sample : M4953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
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Ethanol, 2-(2-b...	10.375	4.3	ng	153182	2	10.569	715416	20.0
Ethyl cycloprop...	12.269	2.5	ng	90801	2	10.569	715416	20.0
1-Decene	14.087	2.9	ng	146370	3	14.428	1024940	20.0
Isopropyl myris...	17.122	2.4	ng	142475	4	17.192	1207680	20.0
n-Hexadecanoic ...	18.098	4.3	ng	260064	4	17.192	1207680	20.0
unknown20.974	20.974	2.2	ng	146072	5	21.298	1305400	20.0
Pentacos-1-ene	21.016	8.2	ng	531705	5	21.298	1305400	20.0
Benzoic acid, 2...	21.075	2.6	ng	168965	5	21.298	1305400	20.0
Squalene	22.545	5.8	ng	293759	6	23.692	1022320	20.0