

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
 Data File : BP008432.D
 Acq On : 16 Dec 2021 01:42
 Operator : CG/JU
 Sample : M5018-19
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP4

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-BP121421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008432.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	316	321	331	rVB	90831	134780	5.26%	0.951%
2	5.340	394	400	417	rBV	765052	1223704	47.73%	8.633%
3	6.940	665	672	695	rBV	650748	1251771	48.82%	8.831%
4	7.740	800	808	818	rBV	198025	324202	12.65%	2.287%
5	8.905	999	1006	1023	rBV	417816	794653	30.99%	5.606%
6	10.540	1276	1284	1298	rBV	217356	416412	16.24%	2.938%
7	13.010	1697	1704	1719	rBV	1048856	1611148	62.84%	11.367%
8	14.393	1932	1939	1955	rBV	329703	545631	21.28%	3.849%
9	14.681	1982	1988	2004	rBV2	73682	189524	7.39%	1.337%
10	15.387	2098	2108	2116	rBV5	15001	36022	1.41%	0.254%
11	15.898	2189	2195	2214	rVB	808437	1351403	52.71%	9.534%
12	16.734	2327	2337	2346	rBV	45083	80966	3.16%	0.571%
13	17.157	2402	2409	2415	rBV	436016	668579	26.08%	4.717%
14	18.028	2551	2557	2559	rBV5	16588	29615	1.16%	0.209%
15	18.063	2559	2563	2570	rVB2	50960	79991	3.12%	0.564%
16	19.187	2750	2754	2760	rVB	41047	57024	2.22%	0.402%
17	19.539	2811	2814	2819	rVB	27612	35553	1.39%	0.251%
18	19.728	2841	2846	2858	rBV	2066130	2563812	100.00%	18.088%
19	20.975	3055	3058	3068	rVB	171291	228836	8.93%	1.614%
20	21.263	3103	3107	3112	rBV	612285	832683	32.48%	5.875%
21	21.381	3122	3127	3138	rBV	547005	807409	31.49%	5.696%
22	23.633	3504	3510	3523	rVB	436835	910447	35.51%	6.423%

Sum of corrected areas: 14174165

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008432.D
Acq On : 16 Dec 2021 01:42
Operator : CG/JU
Sample : M5018-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP4

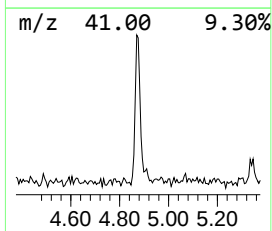
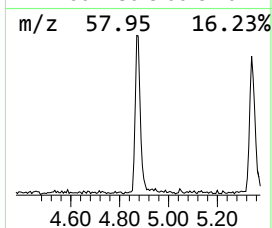
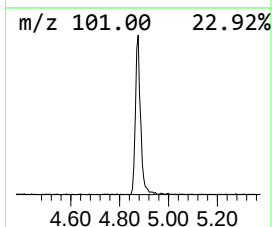
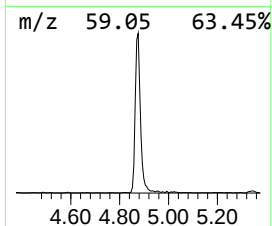
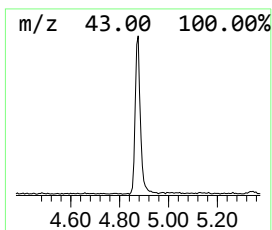
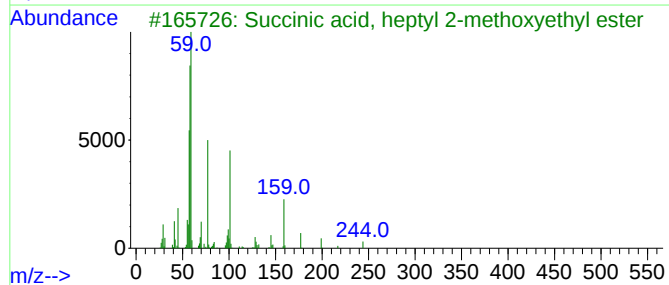
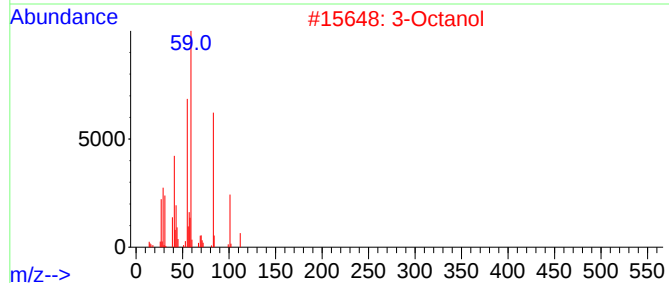
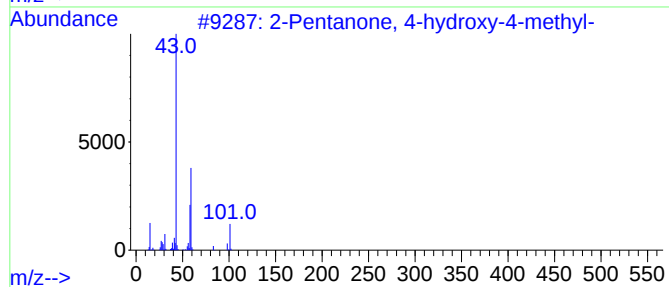
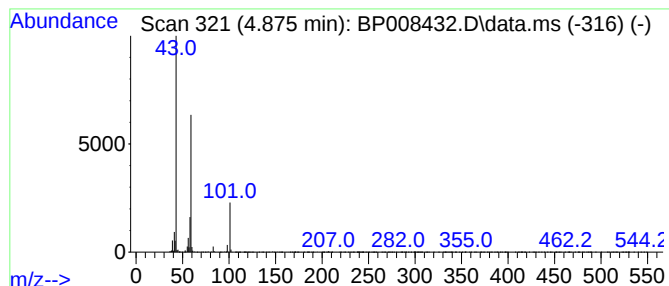
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	8.31 ng	134780	1,4-Dichlorobenzene-d4	7.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008432.D
Acq On : 16 Dec 2021 01:42
Operator : CG/JU
Sample : M5018-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP4

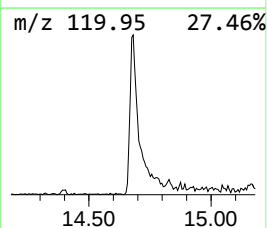
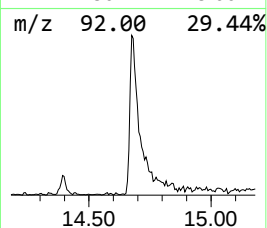
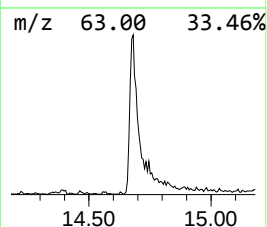
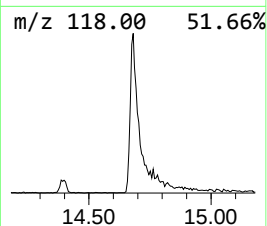
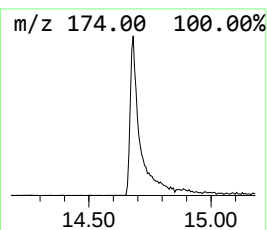
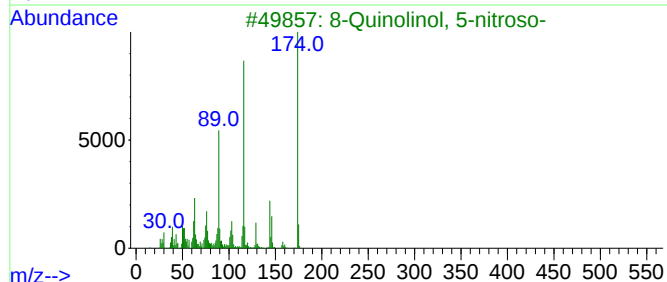
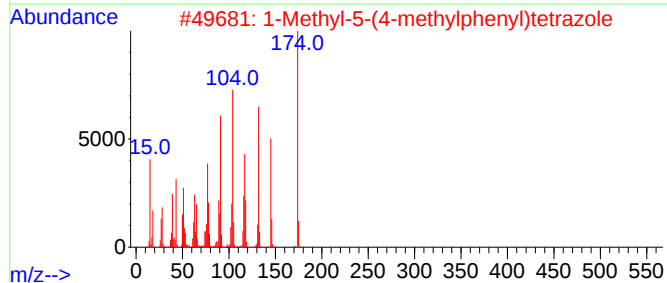
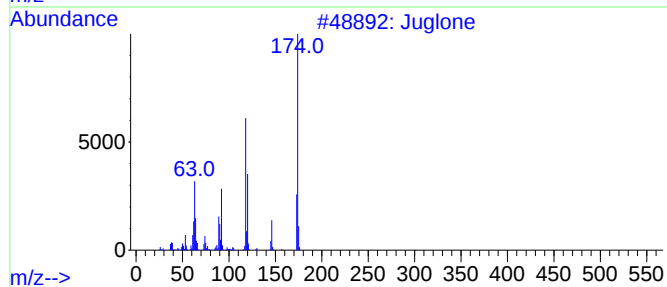
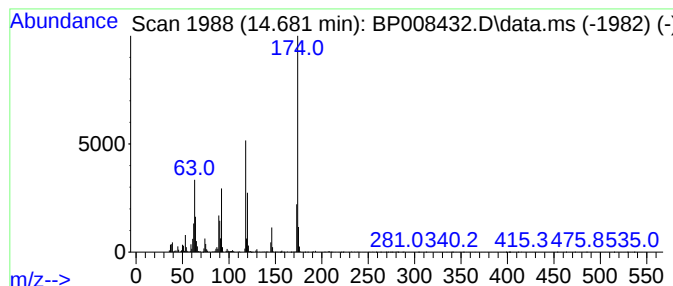
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Juglone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.681	6.95 ng	189524	Acenaphthene-d10	14.393

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Juglone	174	C10H6O3	000481-39-0	95
2			1-Methyl-5-(4-methylphenyl)tetra...	174	C9H10N4	068826-33-5	49
3			8-Quinololinol, 5-nitroso-	174	C9H6N2O2	003565-26-2	43
4			1-(3-Pyridinylmethyl)-3-piperidi...	275	C16H25N3O	1000469-14-7	38
5			Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008432.D
Acq On : 16 Dec 2021 01:42
Operator : CG/JU
Sample : M5018-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP4

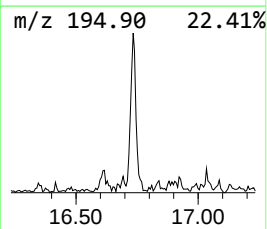
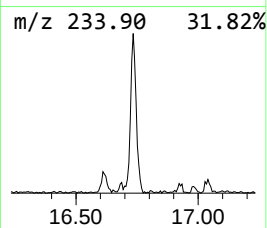
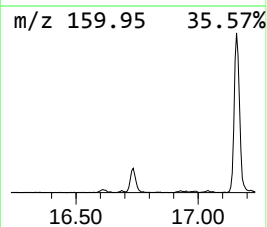
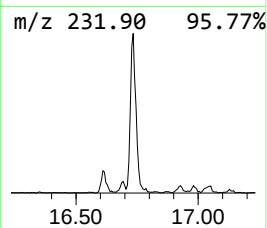
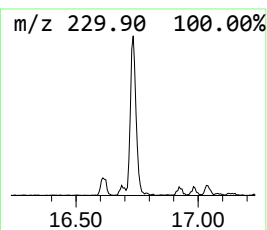
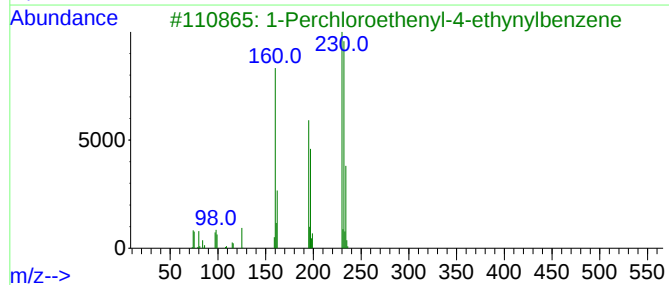
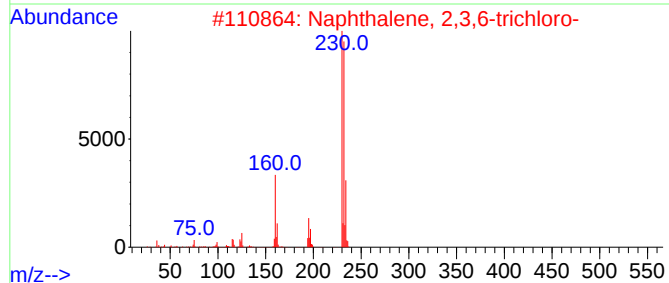
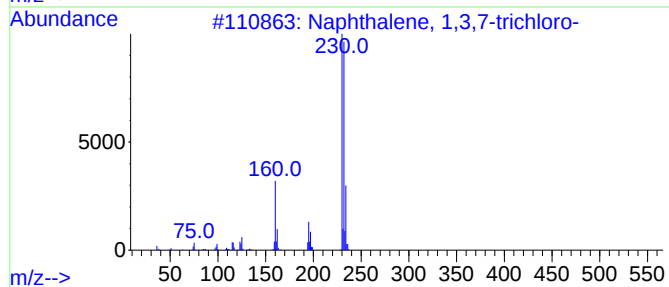
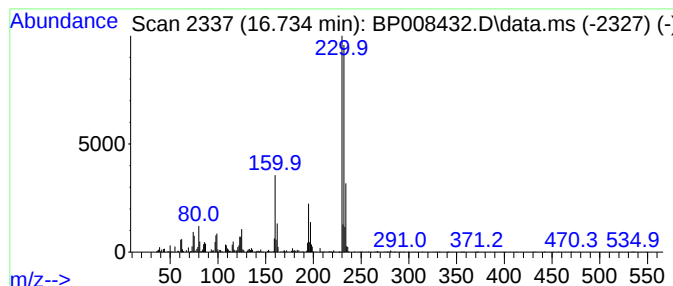
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Naphthalene, 1,3,7-trichloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.734	2.42 ng	80966	Phenanthrene-d10	17.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3,7-trichloro-	230	C10H5Cl3	055720-37-1	99
2			Naphthalene, 2,3,6-trichloro-	230	C10H5Cl3	055720-40-6	98
3			1-Perchloroethenyl-4-ethynylbenzene	230	C10H5Cl3	1000283-76-9	91
4			4-Bromo-6-chloro-1H-indazole	230	C7H4BrClN2	885519-03-9	74
5			4-Bromo-3-chloro-1H-indazole	230	C7H4BrClN2	1000343-46-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008432.D
Acq On : 16 Dec 2021 01:42
Operator : CG/JU
Sample : M5018-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP4

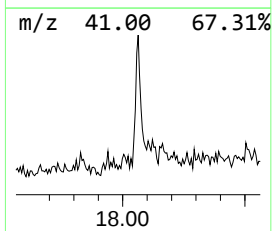
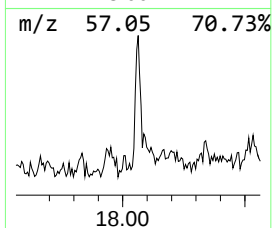
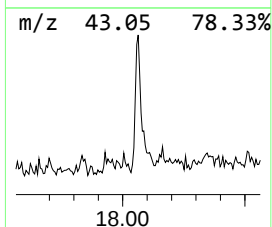
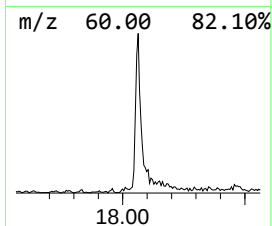
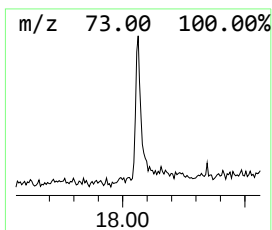
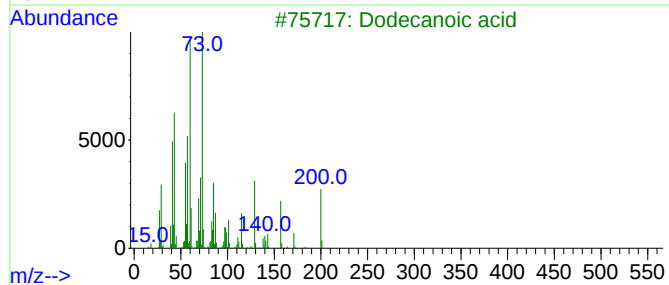
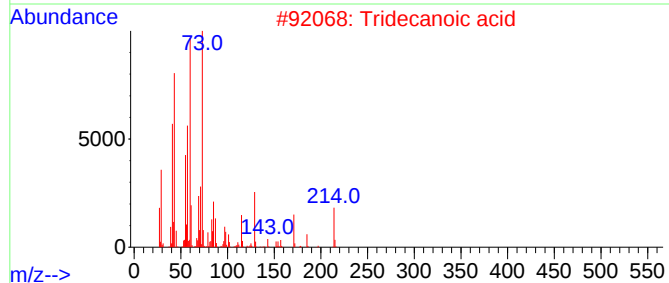
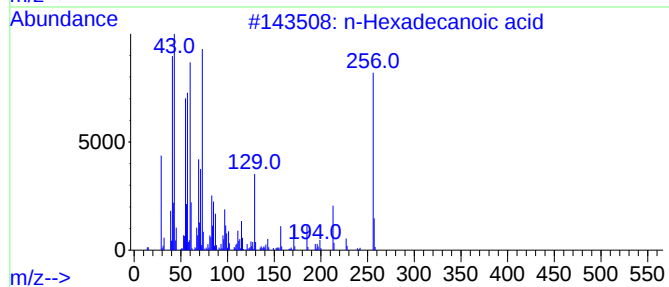
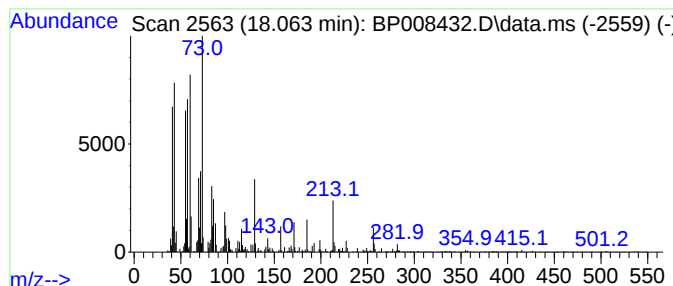
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	2.39 ng	79991	Phenanthrene-d10	17.157

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	90
3			Dodecanoic acid	200	C12H24O2	000143-07-7	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008432.D
Acq On : 16 Dec 2021 01:42
Operator : CG/JU
Sample : M5018-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP4

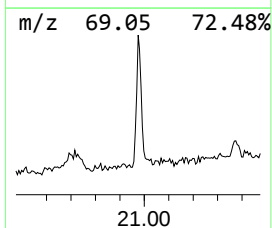
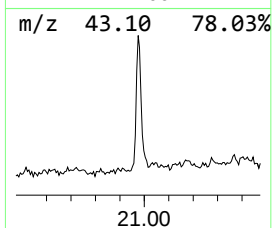
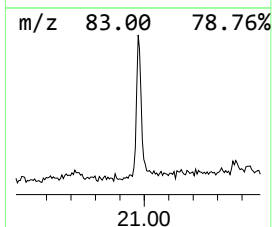
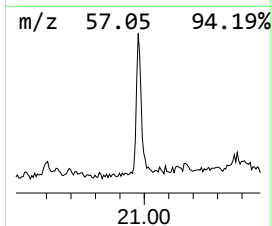
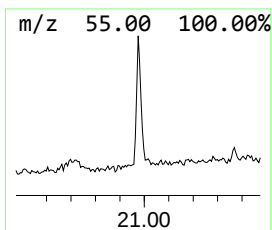
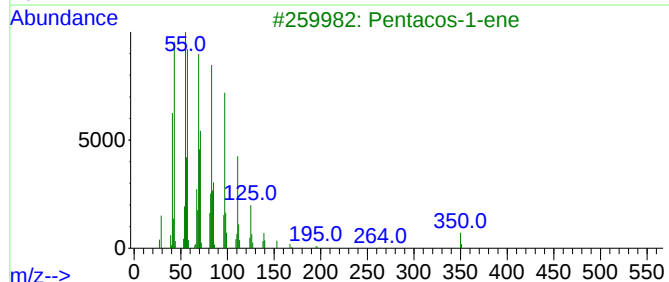
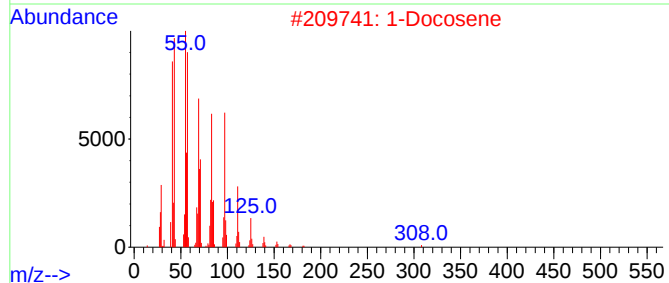
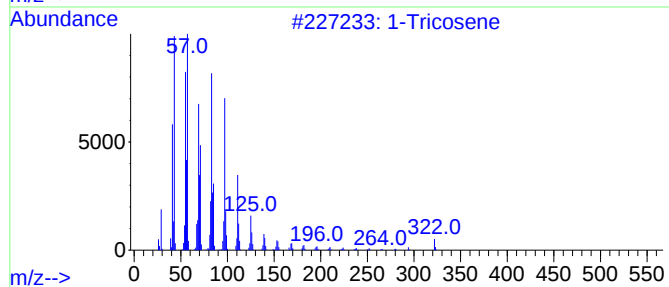
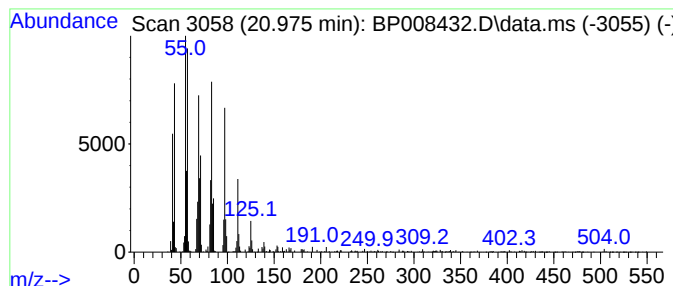
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.975	5.50 ng	228836	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tricosene	322	C23H46	018835-32-0	96
2			1-Docosene	308	C22H44	001599-67-3	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008432.D
Acq On : 16 Dec 2021 01:42
Operator : CG/JU
Sample : M5018-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP4

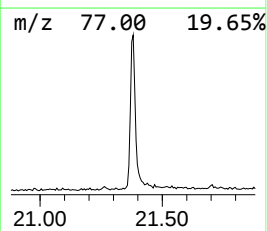
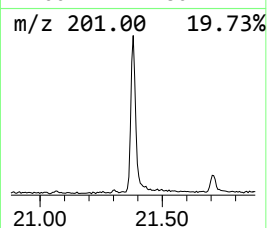
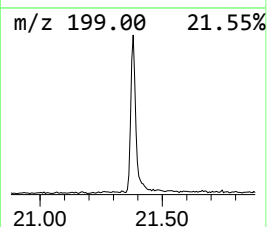
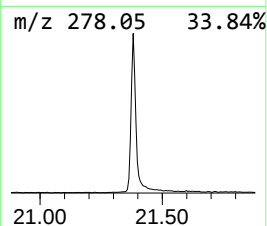
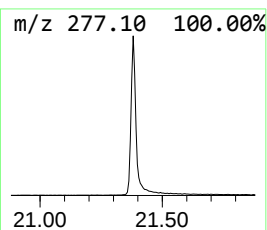
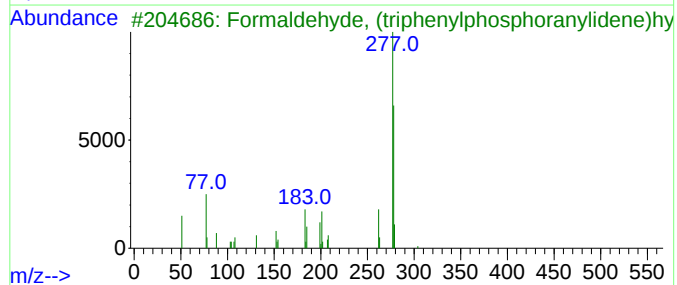
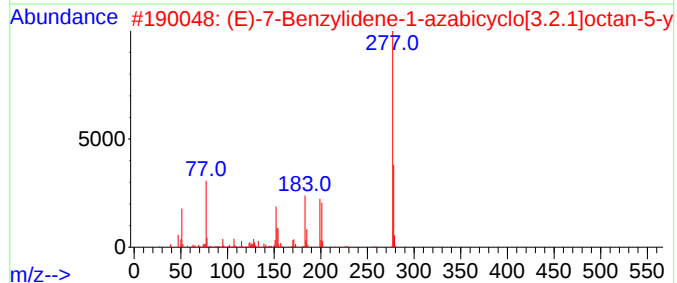
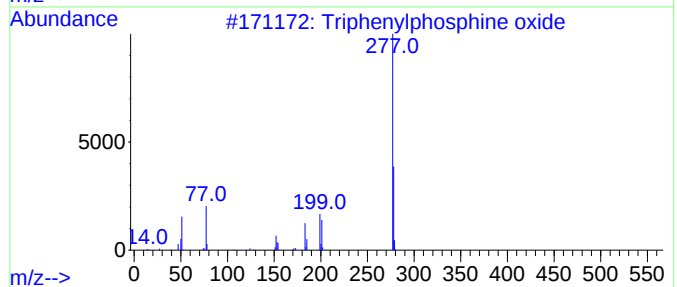
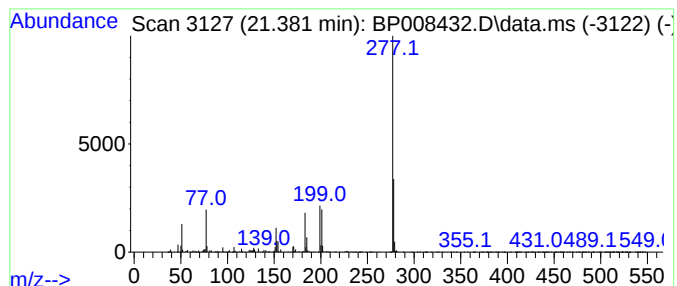
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.381	19.39 ng	807409	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	87
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	40
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28
5			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008432.D
Acq On : 16 Dec 2021 01:42
Operator : CG/JU
Sample : M5018-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.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
2-Pentanone, 4-...	4.875	8.3	ng	134780	1	7.740	324202	20.0
Juglone	14.681	7.0	ng	189524	3	14.393	545631	20.0
Naphthalene, 1,...	16.734	2.4	ng	80966	4	17.157	668579	20.0
n-Hexadecanoic ...	18.063	2.4	ng	79991	4	17.157	668579	20.0
1-Tricosene	20.975	5.5	ng	228836	5	21.269	832683	20.0
Triphenylphosph...	21.381	19.4	ng	807409	5	21.269	832683	20.0