

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
 Data File : BP008411.D
 Acq On : 15 Dec 2021 11:52
 Operator : CG/JU
 Sample : M5076-08
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-18-G

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: BP008411.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	336	rVB	238900	338317	17.14%	2.981%
2	5.346	395	401	422	rVB	546326	886436	44.90%	7.810%
3	5.946	498	503	511	rBV	19623	29839	1.51%	0.263%
4	6.940	666	672	693	rBV	486204	937327	47.48%	8.258%
5	7.740	802	808	818	rBV	174820	293054	14.85%	2.582%
6	8.910	1000	1007	1023	rBV	318177	607245	30.76%	5.350%
7	10.540	1276	1284	1299	rBV	192472	365445	18.51%	3.220%
8	13.016	1698	1705	1723	rBV	757120	1209886	61.29%	10.660%
9	14.398	1933	1940	1948	rBV	291018	461401	23.37%	4.065%
10	15.904	2189	2196	2214	rBV	397022	791872	40.11%	6.977%
11	17.092	2392	2398	2403	rBV3	15240	25453	1.29%	0.224%
12	17.163	2403	2410	2424	rVV	354976	577359	29.25%	5.087%
13	18.069	2560	2564	2571	rBV3	43434	89075	4.51%	0.785%
14	18.127	2572	2574	2583	rVB	13957	21748	1.10%	0.192%
15	18.792	2680	2687	2689	rBV2	29636	56965	2.89%	0.502%
16	19.310	2771	2775	2785	rBV4	26991	56963	2.89%	0.502%
17	19.551	2812	2816	2820	rVB3	15480	21735	1.10%	0.191%
18	19.733	2841	2847	2856	rBV	1580126	1974028	100.00%	17.392%
19	20.051	2896	2901	2914	rVB3	53507	145178	7.35%	1.279%
20	20.974	3054	3058	3067	rVB	122190	212538	10.77%	1.873%
21	21.269	3103	3108	3118	rBV	521692	741211	37.55%	6.530%
22	21.380	3123	3127	3139	rBV	452132	821292	41.60%	7.236%
23	23.633	3505	3510	3521	rVB2	323027	685802	34.74%	6.042%

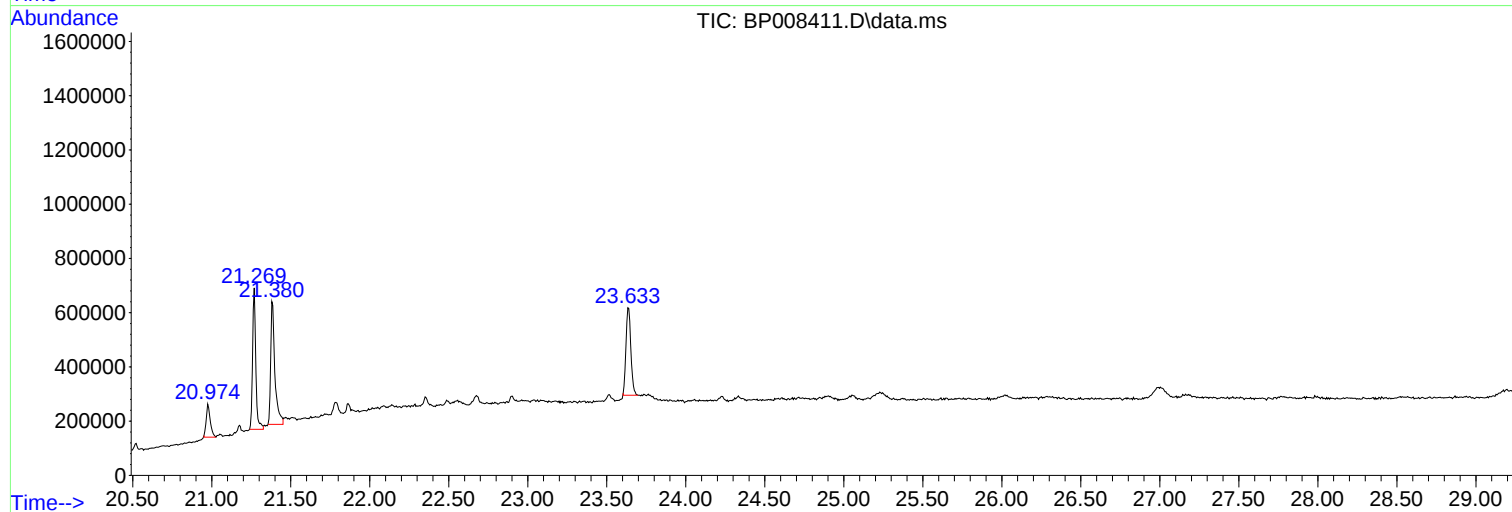
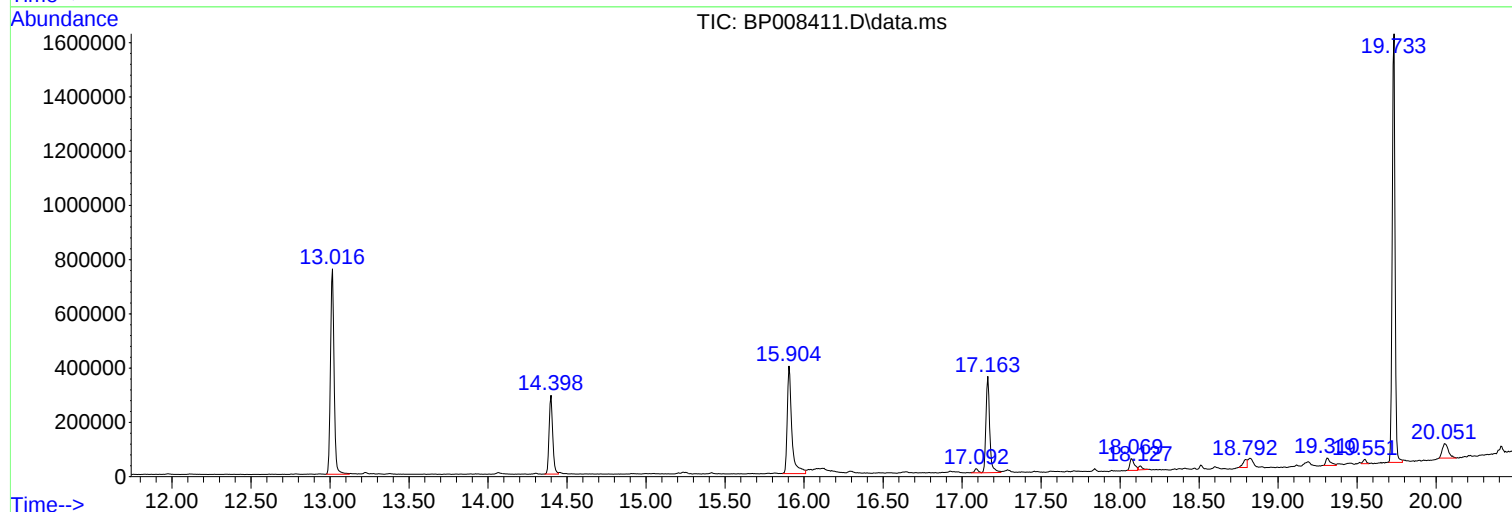
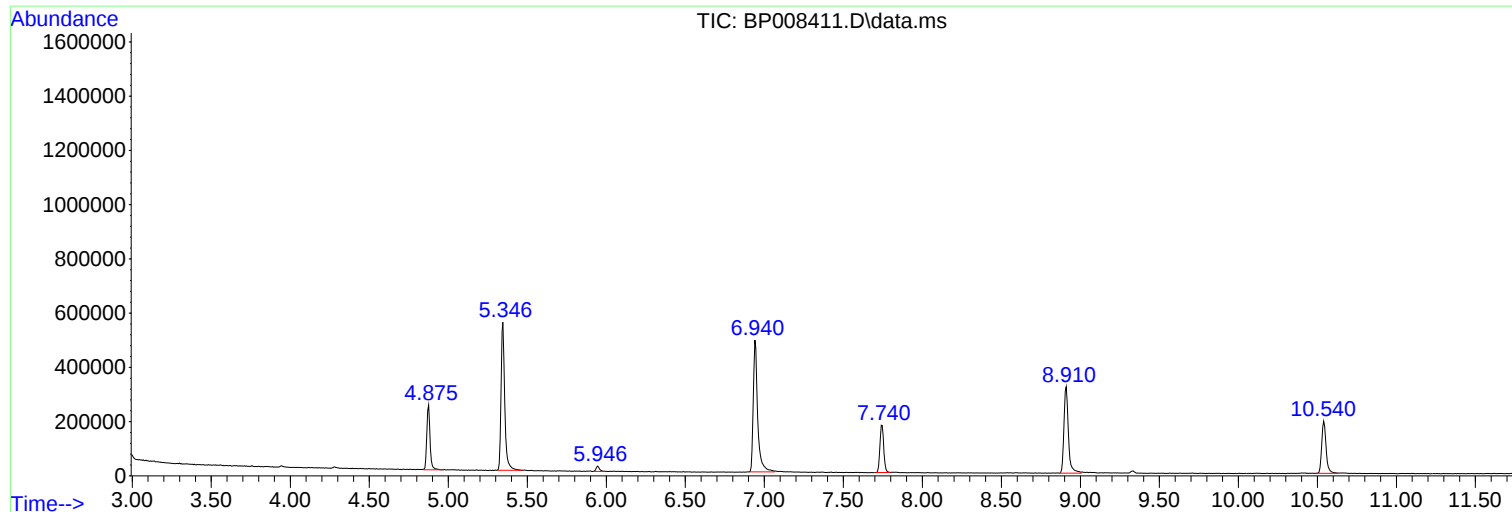
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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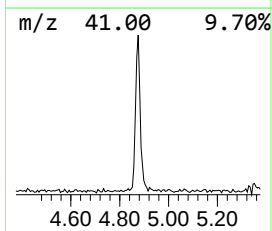
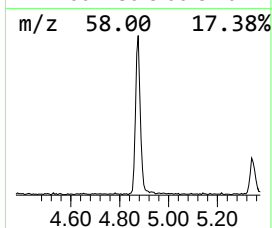
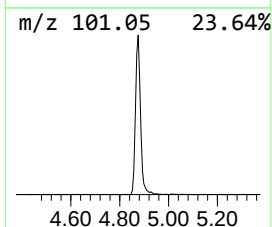
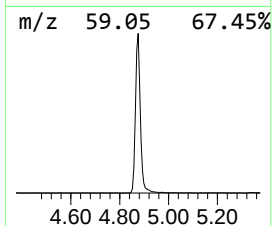
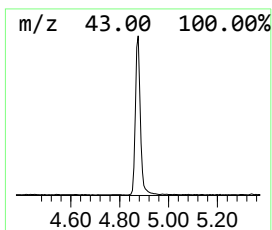
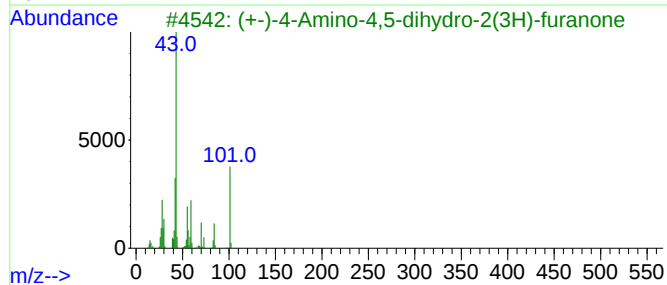
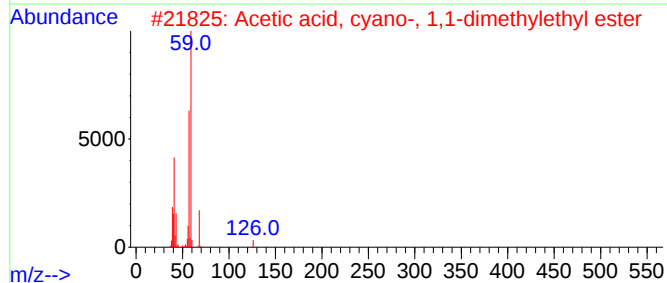
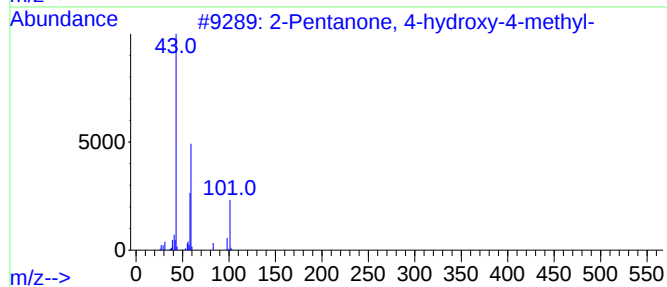
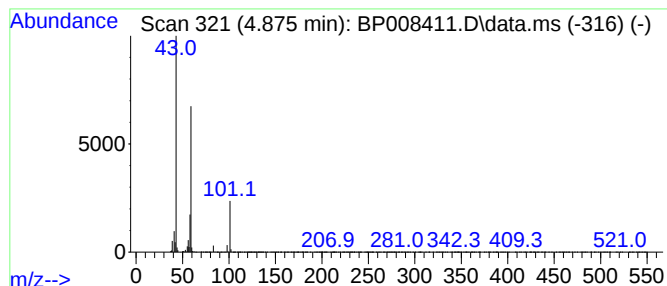
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.875	23.09 ng	338317	1,4-Dichlorobenzene-d4			7.746

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	23
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2		016504-58-8	9
4	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O		000628-81-9	9



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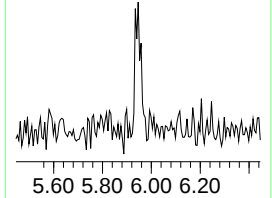
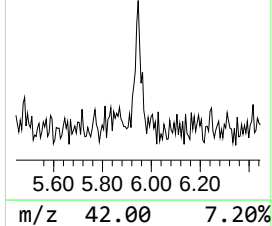
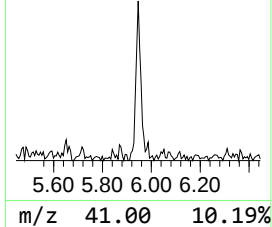
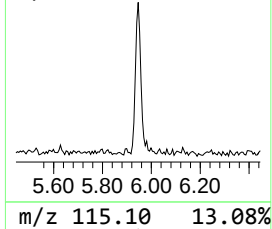
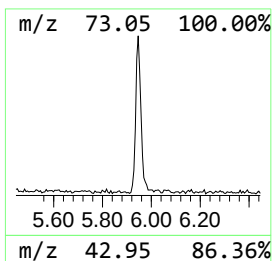
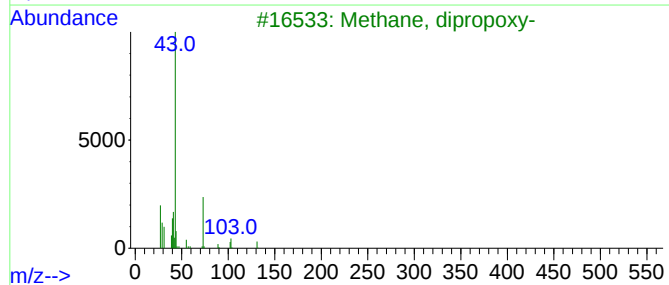
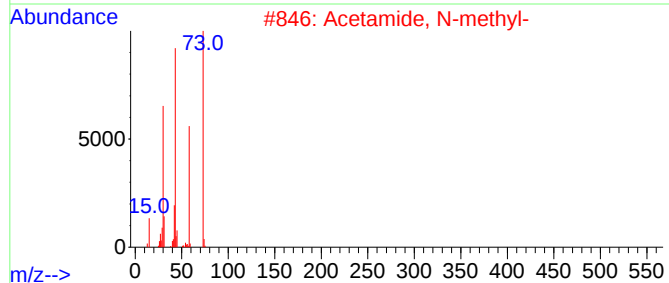
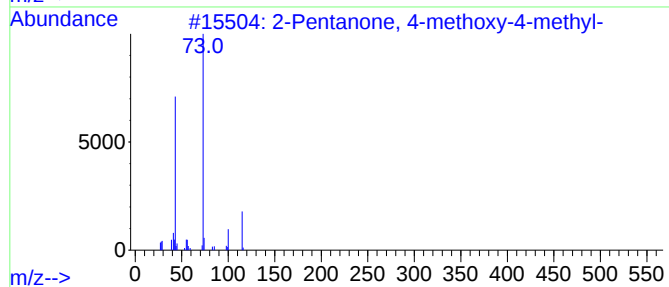
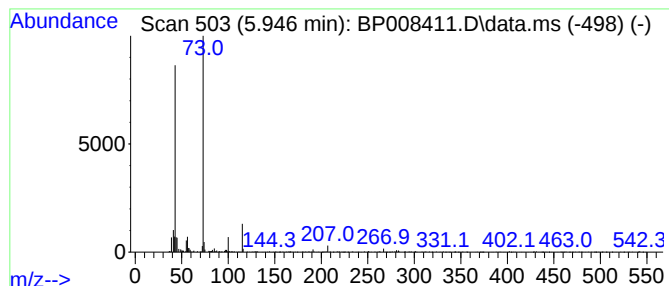
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.946	2.04 ng	29839	1,4-Dichlorobenzene-d4		7.746	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	59
2	Acetamide, N-methyl-		73	C3H7NO	000079-16-3	43
3	Methane, dipropoxy-		132	C7H16O2	000505-84-0	38
4	2-Acetamido-N-methylacetamide		130	C5H10N2O2	007606-79-3	35
5	3-Hexanol, acetate		144	C8H16O2	040780-64-1	25



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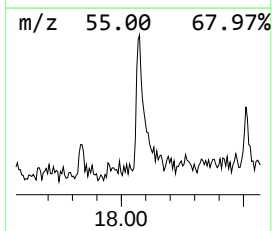
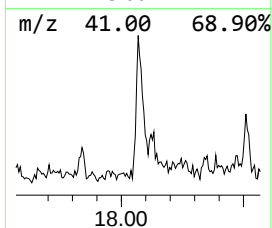
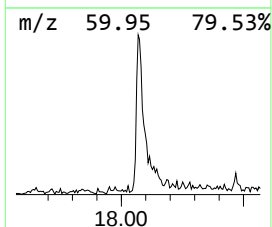
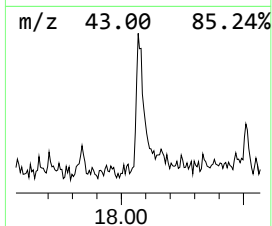
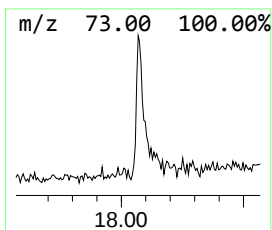
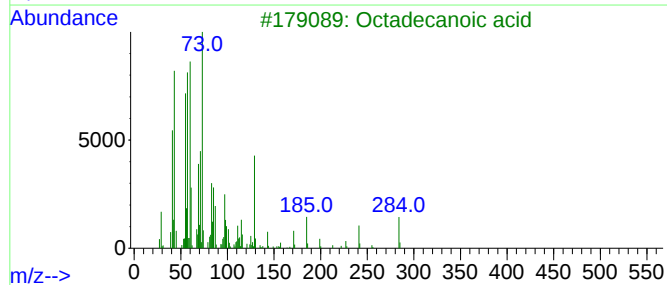
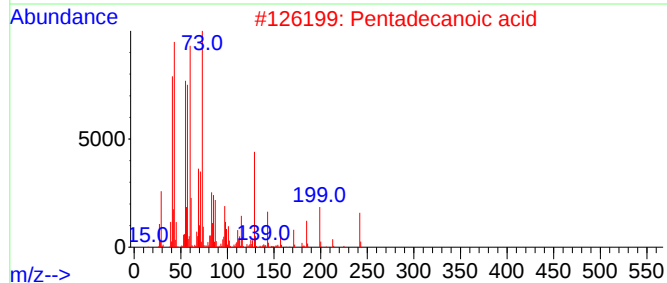
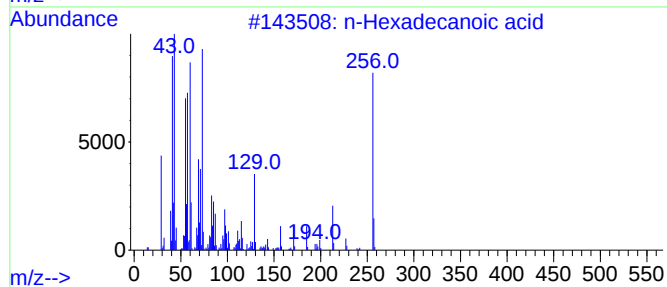
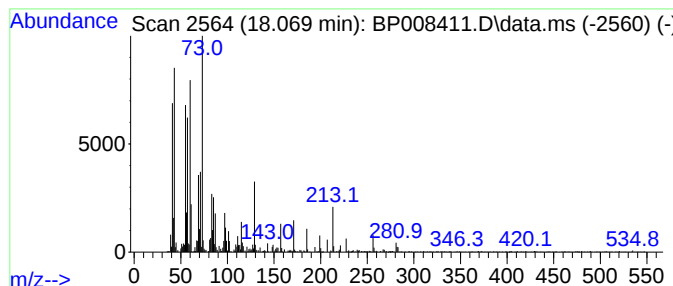
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.069	3.09 ng	89075	Phenanthrene-d10	17.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Octadecanoic acid	284	C18H36O2	000057-11-4	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	83
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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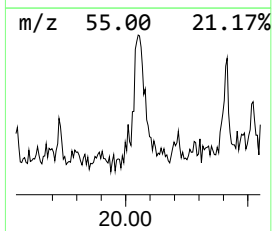
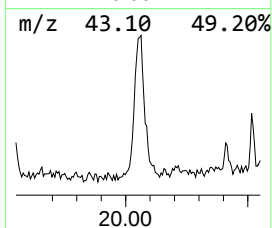
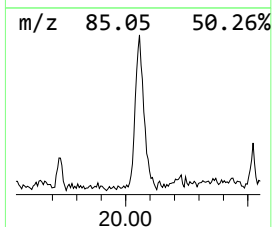
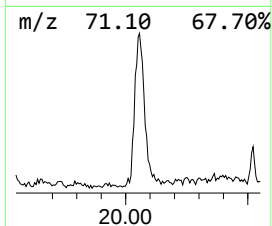
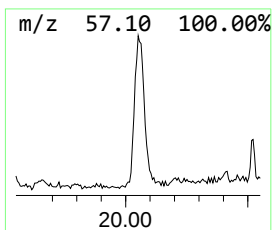
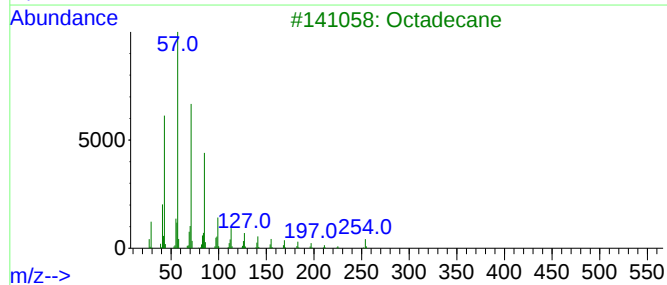
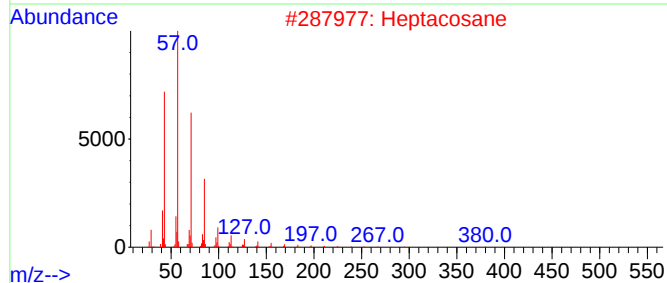
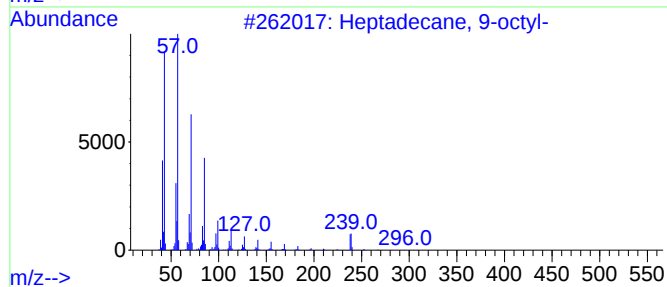
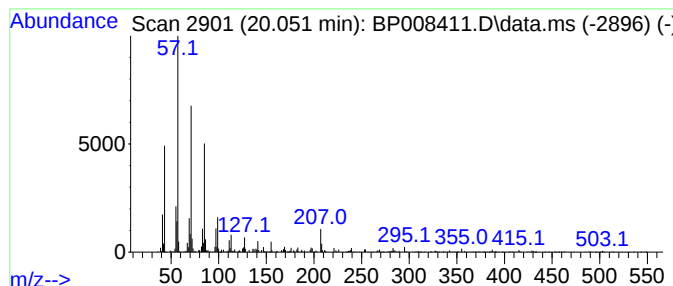
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Peak Number 4 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.051	3.92 ng	145178	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
2			Heptacosane	380	C27H56	000593-49-7	92
3			Octadecane	254	C18H38	000593-45-3	90
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	89
5			Tritriacontane	465	C33H68	000630-05-7	87



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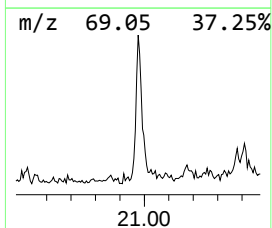
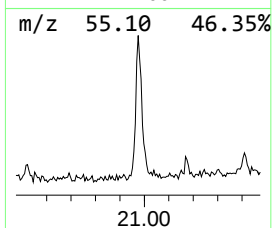
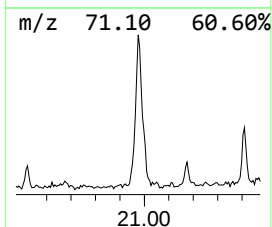
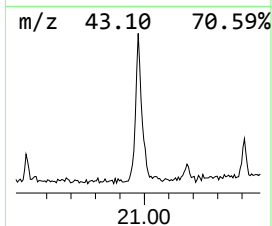
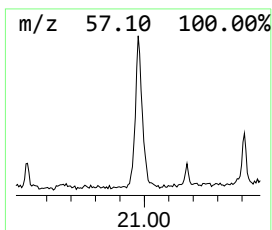
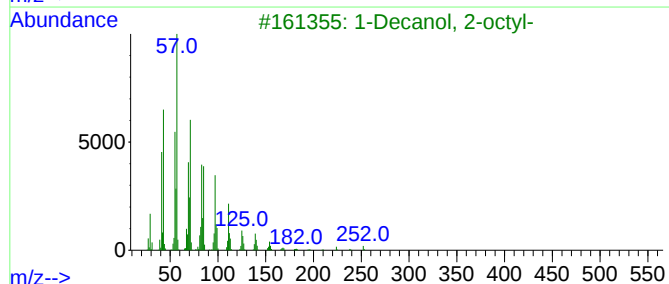
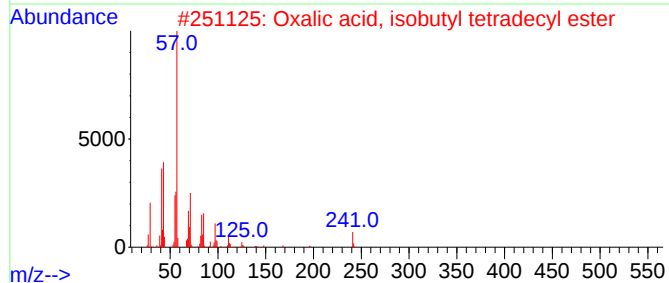
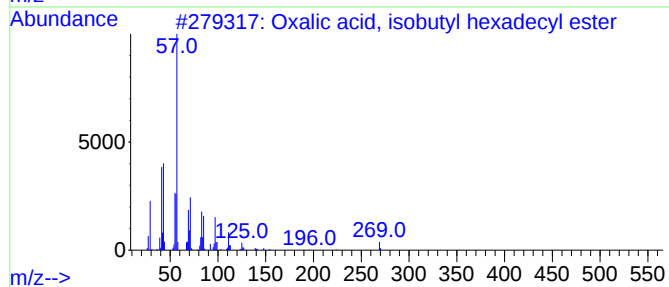
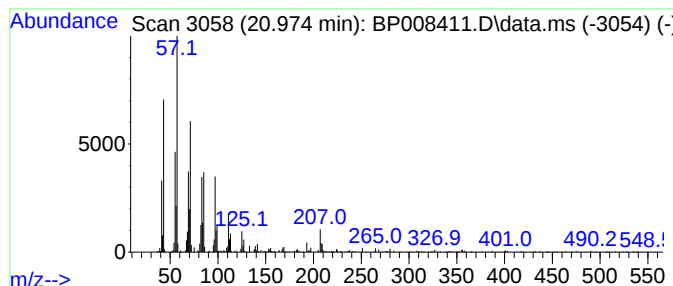
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Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	5.73 ng	212538	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
2			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	87
3			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	87
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	87
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	83



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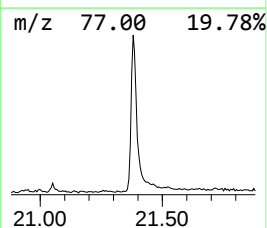
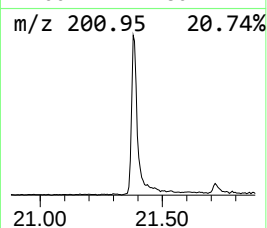
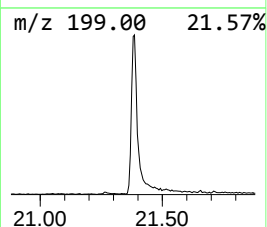
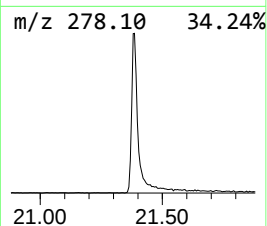
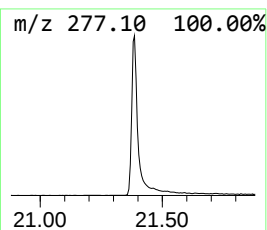
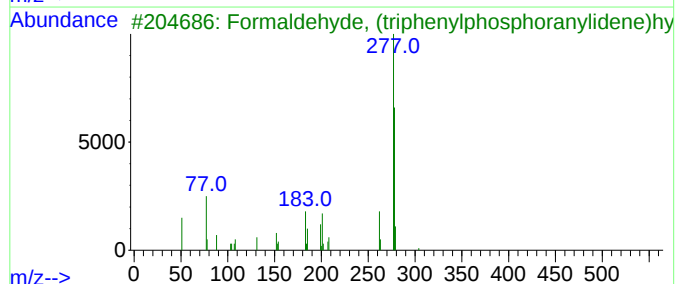
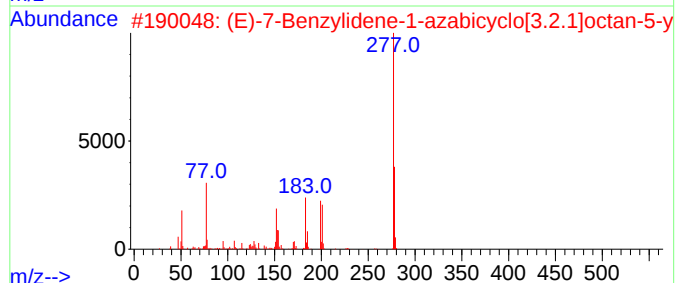
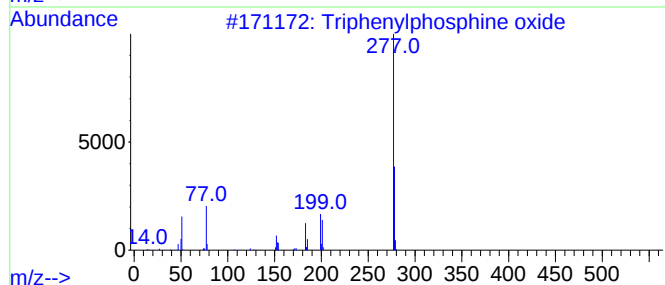
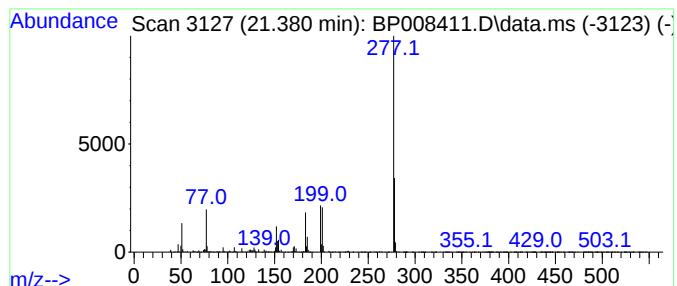
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.380	22.16 ng	821292	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	87
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	42
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28
5			5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008411.D
Acq On : 15 Dec 2021 11:52
Operator : CG/JU
Sample : M5076-08
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-18-G

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	23.1	ng	338317	1	7.746	293054	20.0
2-Pentanone, 4-...	5.946	2.0	ng	29839	1	7.746	293054	20.0
n-Hexadecanoic ...	18.069	3.1	ng	89075	4	17.163	577359	20.0
Heptadecane, 9-...	20.051	3.9	ng	145178	5	21.269	741211	20.0
Oxalic acid, is...	20.974	5.7	ng	212538	5	21.269	741211	20.0
Triphenylphosph...	21.380	22.2	ng	821292	5	21.269	741211	20.0