

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
 Data File : BP008280.D
 Acq On : 08 Dec 2021 15:00
 Operator : CG/JU
 Sample : M4953-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A1513

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: BP008280.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	399	405	420	rBV	580447	855559	21.11%	4.330%
2	6.963	667	676	697	rVB	311739	601897	14.85%	3.046%
3	7.775	804	814	821	rBV	307058	501953	12.39%	2.540%
4	8.940	1004	1012	1024	rBV	1037764	1744115	43.04%	8.827%
5	9.369	1074	1085	1090	rBV	28511	46283	1.14%	0.234%
6	10.381	1248	1257	1275	rBV2	34434	92348	2.28%	0.467%
7	10.569	1281	1289	1299	rBV	362064	632203	15.60%	3.200%
8	13.046	1702	1710	1723	rBV	2424492	3564494	87.97%	18.040%
9	14.093	1882	1888	1896	rBV3	29735	60744	1.50%	0.307%
10	14.428	1938	1945	1954	rBV	514504	757399	18.69%	3.833%
11	15.257	2078	2086	2091	rBV2	69258	150275	3.71%	0.761%
12	15.928	2194	2200	2209	rBV	1114678	1656804	40.89%	8.385%
13	17.122	2398	2403	2408	rVB	50274	61983	1.53%	0.314%
14	17.192	2408	2415	2423	rBV	548347	789249	19.48%	3.994%
15	17.492	2461	2466	2476	rVB4	20416	45594	1.13%	0.231%
16	17.622	2480	2488	2493	rBV6	17968	44101	1.09%	0.223%
17	18.092	2564	2568	2575	rBV	91843	142370	3.51%	0.721%
18	18.157	2576	2579	2584	rVB	35641	48380	1.19%	0.245%
19	18.504	2634	2638	2643	rBV2	91677	104835	2.59%	0.531%
20	19.333	2776	2779	2788	rVB5	35924	48964	1.21%	0.248%
21	19.769	2847	2853	2862	rBV	3284416	4052088	100.00%	20.508%
22	20.445	2964	2968	2974	rBV	132594	166362	4.11%	0.842%
23	20.516	2977	2980	2984	rVV	72553	80310	1.98%	0.406%
24	20.974	3054	3058	3061	rBV	58103	90895	2.24%	0.460%
25	21.016	3061	3065	3072	rVV2	240589	380325	9.39%	1.925%
26	21.080	3073	3076	3084	rVB	96716	129729	3.20%	0.657%
27	21.210	3095	3098	3104	rBV	147587	178391	4.40%	0.903%
28	21.298	3107	3113	3117	rBV2	771364	1127151	27.82%	5.705%
29	21.339	3117	3120	3128	rVB	112074	174576	4.31%	0.884%
30	22.133	3252	3255	3260	rVB	80933	104634	2.58%	0.530%
31	22.545	3321	3325	3330	rBV	157825	214504	5.29%	1.086%
32	23.692	3514	3520	3530	rVB	546387	1110299	27.40%	5.619%

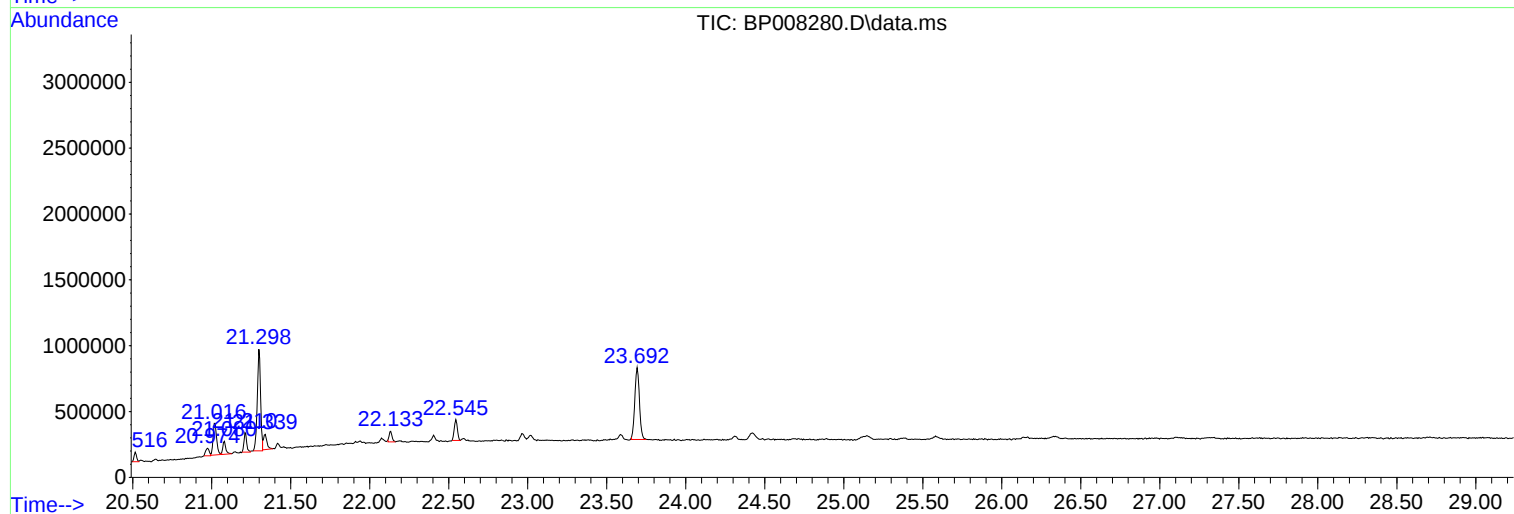
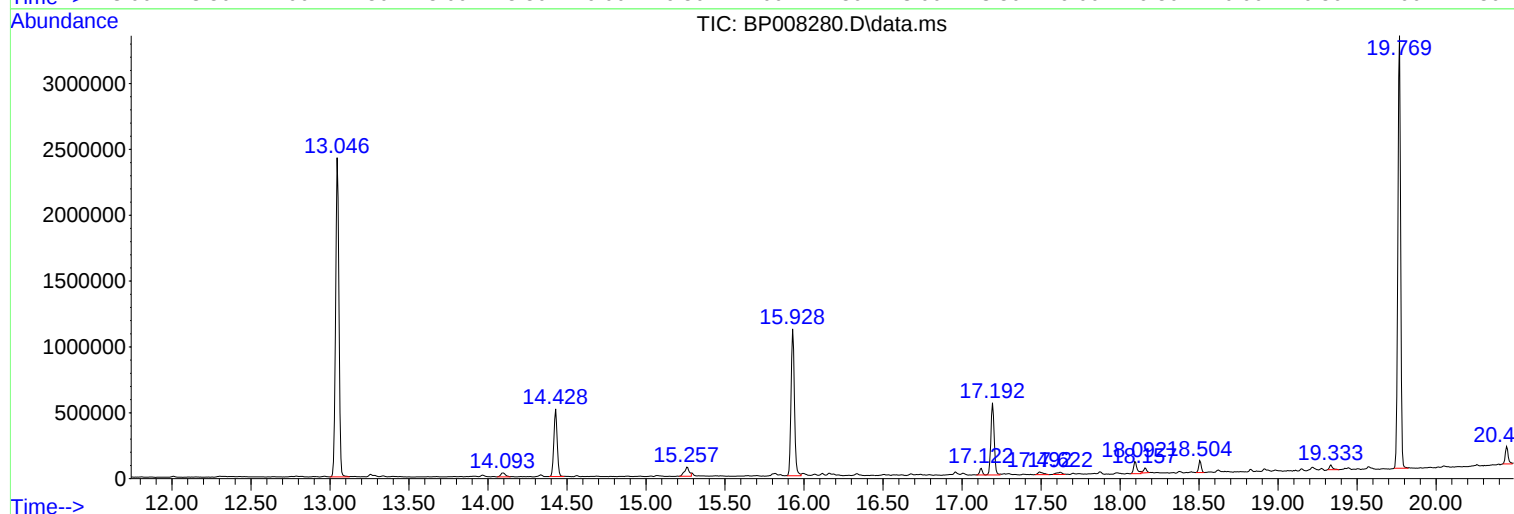
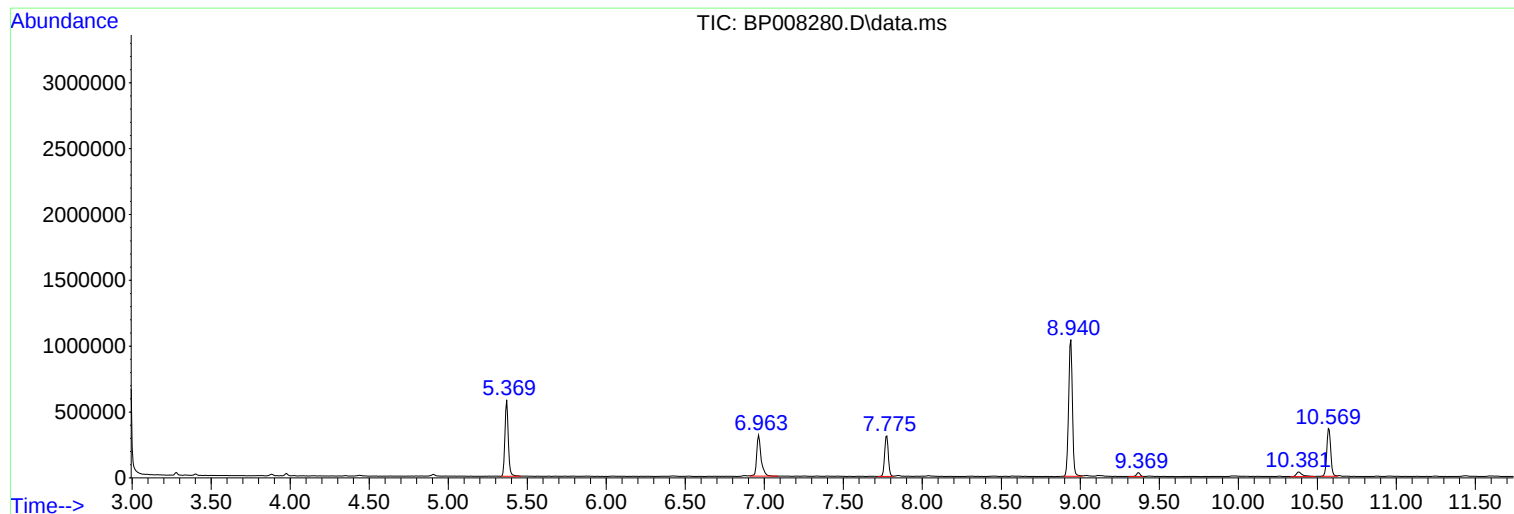
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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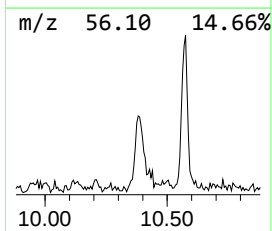
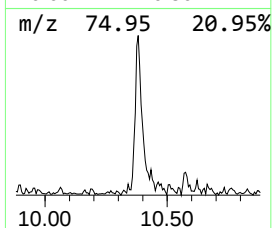
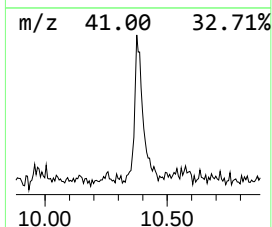
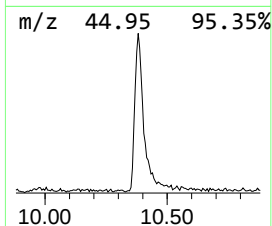
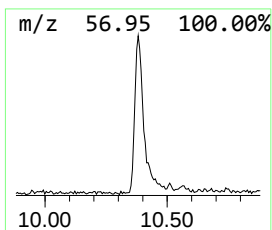
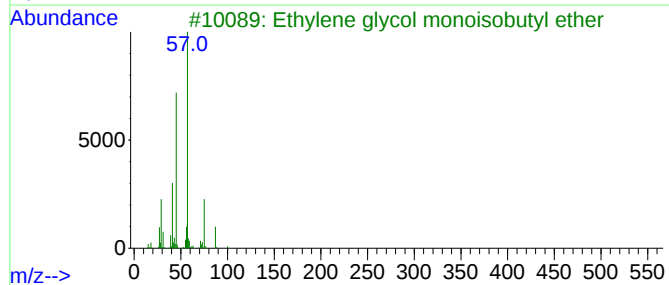
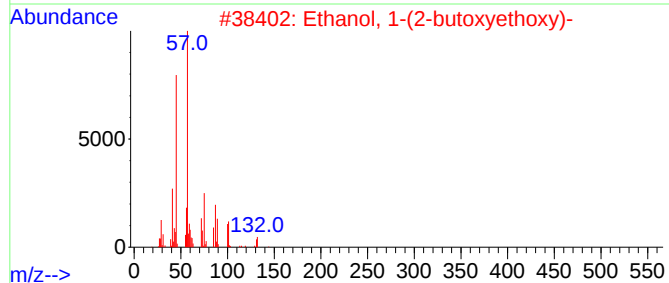
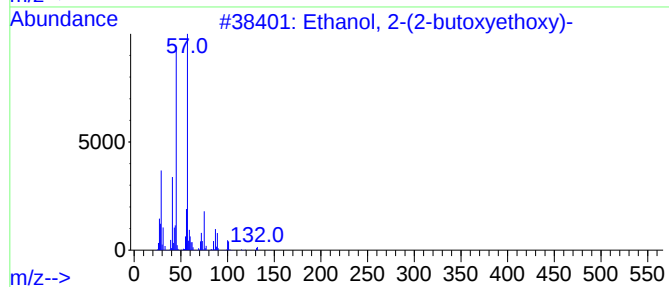
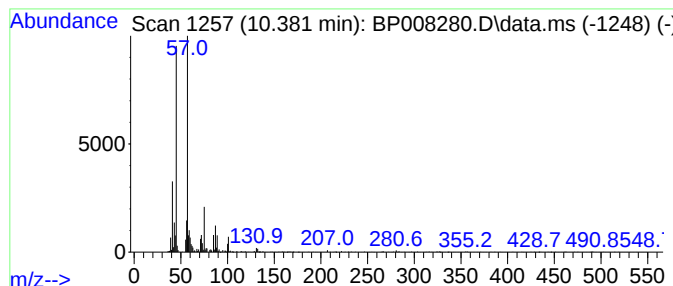
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.381	2.92 ng	92348	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	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Hexaethylene glycol	282	C12H26O7	002615-15-8	50



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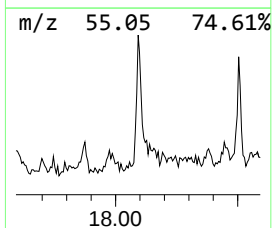
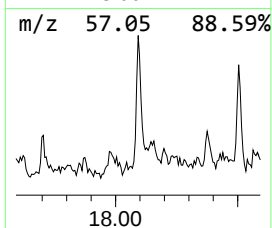
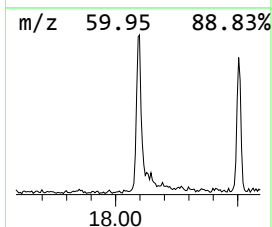
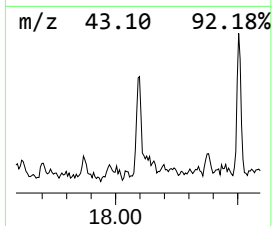
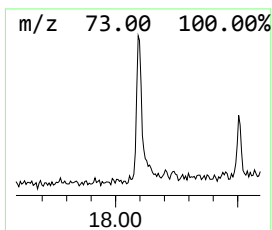
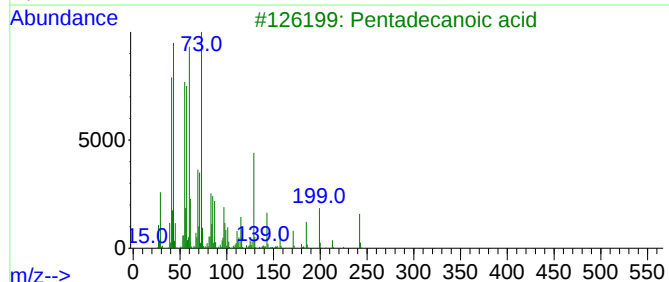
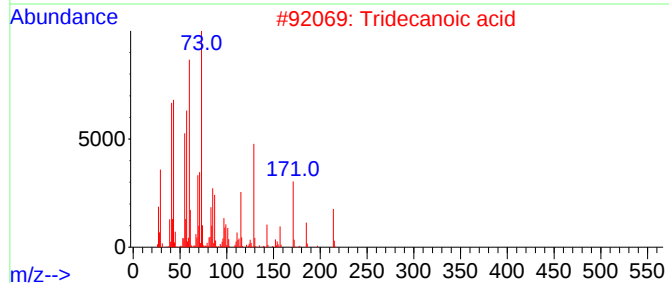
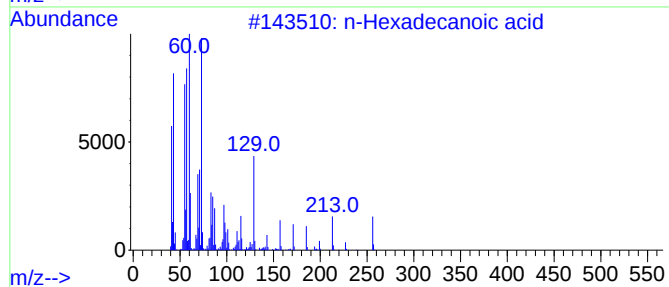
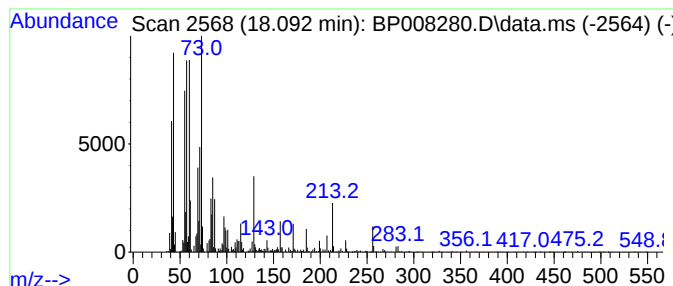
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	3.61 ng	142370	Phenanthrene-d10	17.192

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	62



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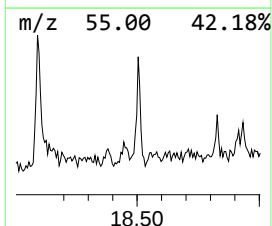
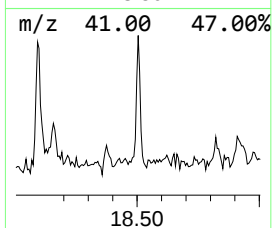
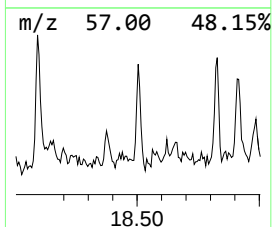
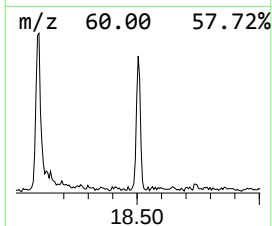
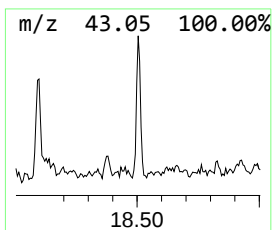
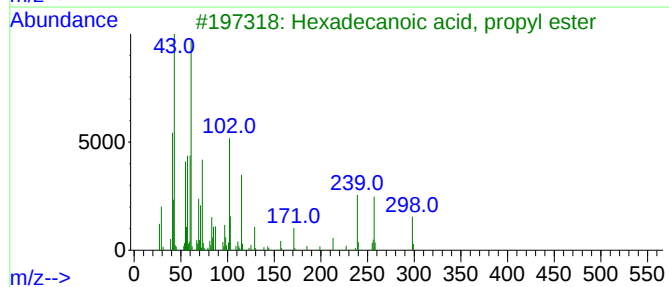
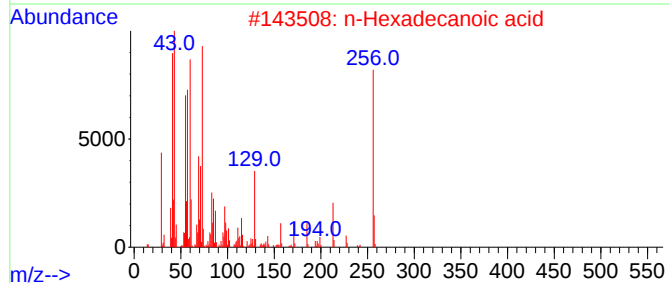
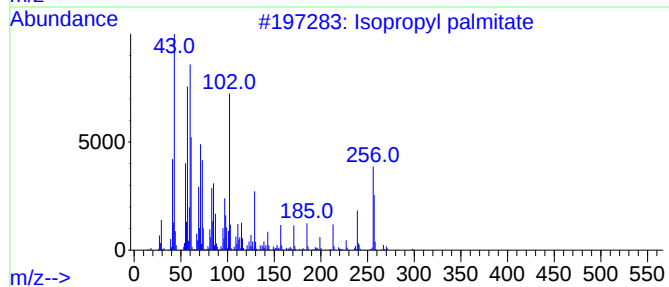
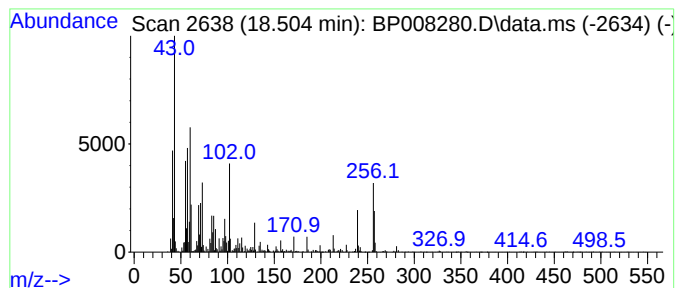
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Peak Number 3 Isopropyl palmitate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.504	2.66 ng	104835	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3			Hexadecanoic acid, propyl ester	298	C19H38O2	002239-78-3	62
4			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	27
5			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	27



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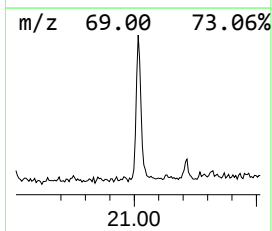
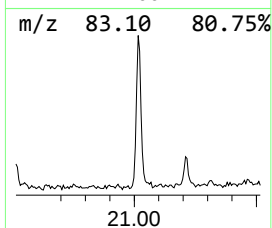
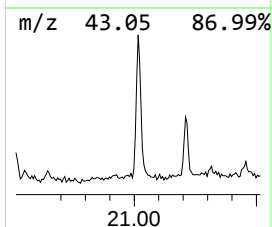
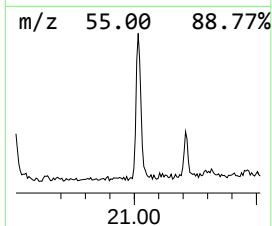
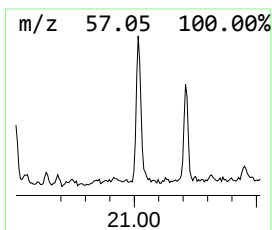
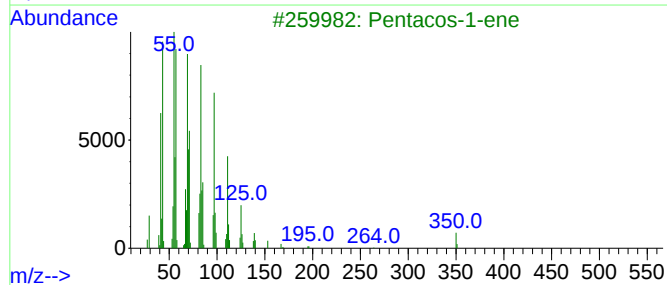
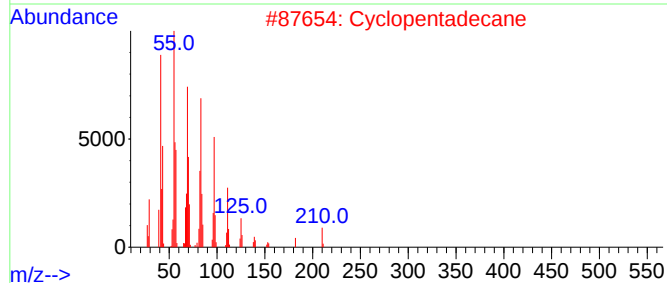
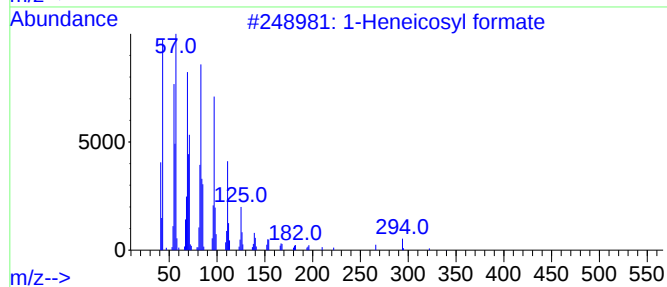
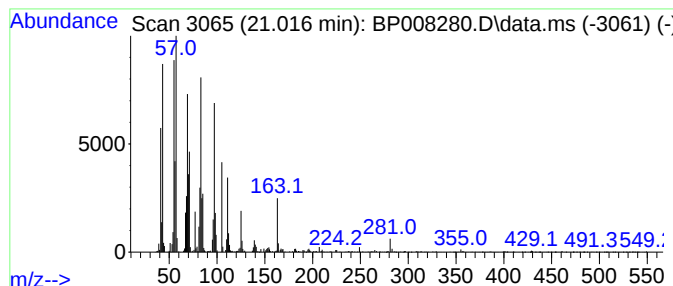
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Peak Number 4 1-Heneicosyl formate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.016	6.75 ng	380325	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	99
2			Cyclopentadecane	210	C15H30	000295-48-7	93
3			Pentacos-1-ene	350	C25H50	016980-85-1	93
4			1-Tetracosene	336	C24H48	010192-32-2	91
5			1-Hexacosene	364	C26H52	018835-33-1	90



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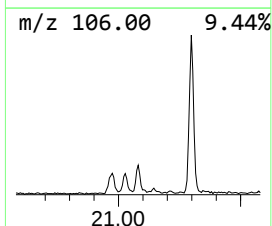
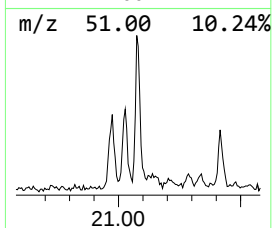
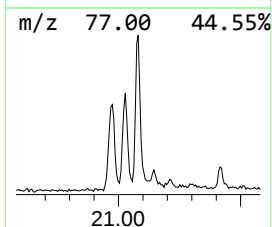
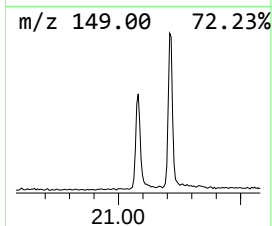
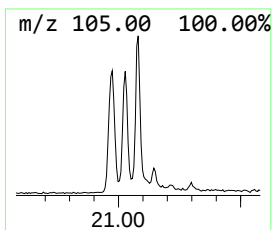
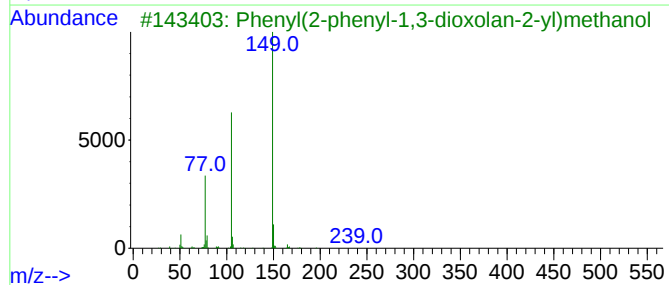
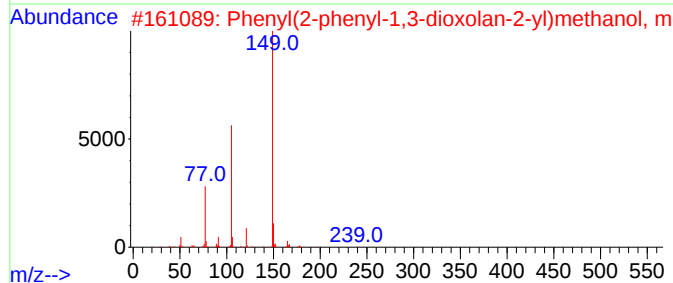
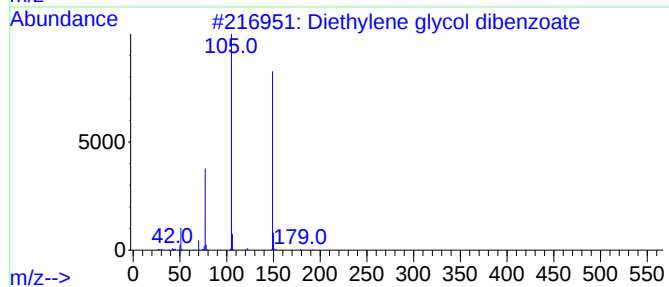
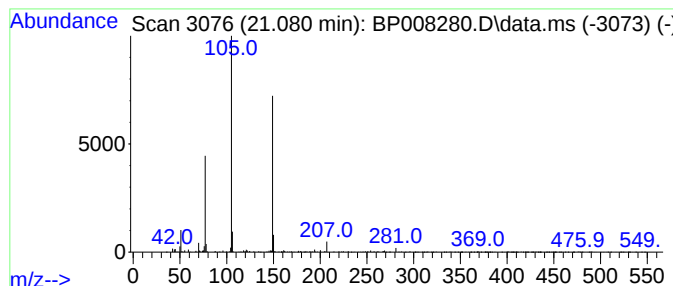
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	2.30 ng	129729	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	72
3			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	72
4			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	53
5			N-(3-Phenyl-1,2,4-thiadiazol-5-y...	281	C15H11N3OS	017280-75-0	43



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A1513

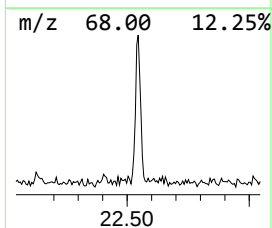
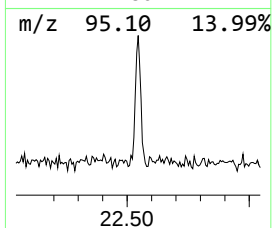
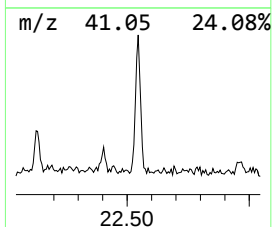
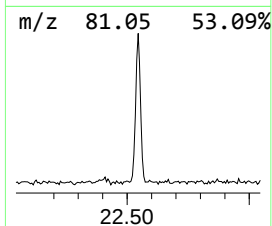
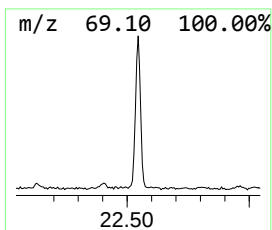
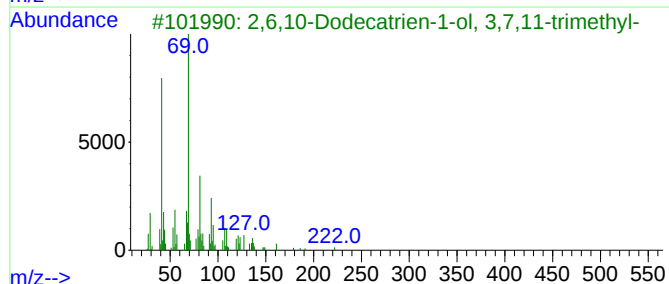
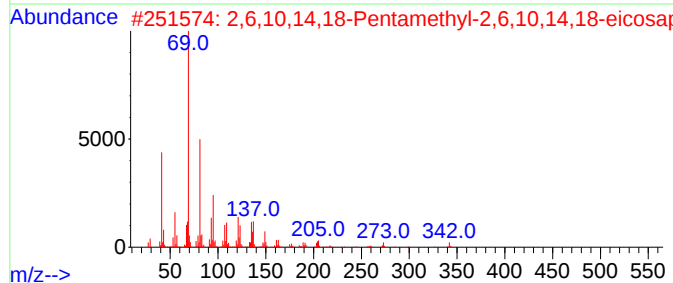
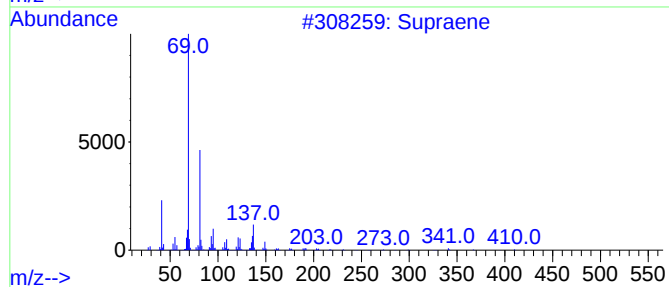
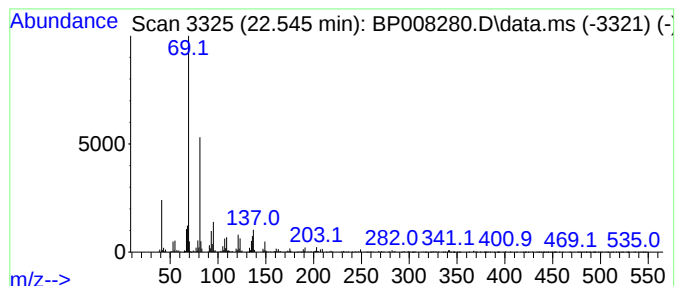
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.545	3.86 ng	214504	Perylene-d12	23.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	74
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
4			trans-Farnesol	222	C15H26O	000106-28-5	59
5			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008280.D
Acq On : 08 Dec 2021 15:00
Operator : CG/JU
Sample : M4953-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A1513

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.381	2.9	ng	92348	2	10.569	632203	20.0
n-Hexadecanoic ...	18.092	3.6	ng	142370	4	17.192	789249	20.0
Isopropyl palmi...	18.504	2.7	ng	104835	4	17.192	789249	20.0
1-Heneicosyl fo...	21.016	6.8	ng	380325	5	21.298	1127150	20.0
Diethylene glyc...	21.080	2.3	ng	129729	5	21.298	1127150	20.0
Supraene	22.545	3.9	ng	214504	6	23.692	1110300	20.0