

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
 Data File : BF129659.D
 Acq On : 09 Aug 2022 10:38
 Operator : CG\JU
 Sample : PB146816BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB146816BL

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_F\Methods\8270-BF072522.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129659.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.487	539	544	547	rBV	5295031	5373466	67.79%	11.825%
2	6.493	710	715	718	rBV	4547894	5506556	69.47%	12.118%
3	6.840	770	774	777	rBV	1424036	1176007	14.84%	2.588%
4	7.410	865	871	874	rBV	3392311	3738531	47.17%	8.227%
5	8.122	987	992	995	rBV	1880253	1652928	20.85%	3.637%
6	9.198	1169	1175	1178	rBV	6646324	7204565	90.90%	15.854%
7	9.881	1285	1291	1294	rBV	2304303	2017552	25.45%	4.440%
8	10.680	1420	1427	1430	rBV	4495733	4658570	58.78%	10.252%
9	11.369	1540	1544	1548	rVB	2421590	2048451	25.84%	4.508%
10	12.763	1777	1781	1785	rVB	303652	237999	3.00%	0.524%
11	12.963	1809	1815	1818	rBV	7634002	7926055	100.00%	17.442%
12	13.469	1897	1901	1904	rBV	205156	180275	2.27%	0.397%
13	14.016	1990	1994	1998	rBV	1743984	1550818	19.57%	3.413%
14	14.104	2004	2009	2014	rBV	161009	174978	2.21%	0.385%
15	15.104	2174	2179	2195	rVB	120699	335699	4.24%	0.739%
16	15.492	2239	2245	2251	rVB	968322	1249769	15.77%	2.750%
17	15.910	2312	2316	2321	rBV2	63155	82830	1.05%	0.182%
18	16.410	2398	2401	2407	rVB2	50070	81528	1.03%	0.179%
19	16.998	2497	2501	2516	rVB4	73442	245631	3.10%	0.541%

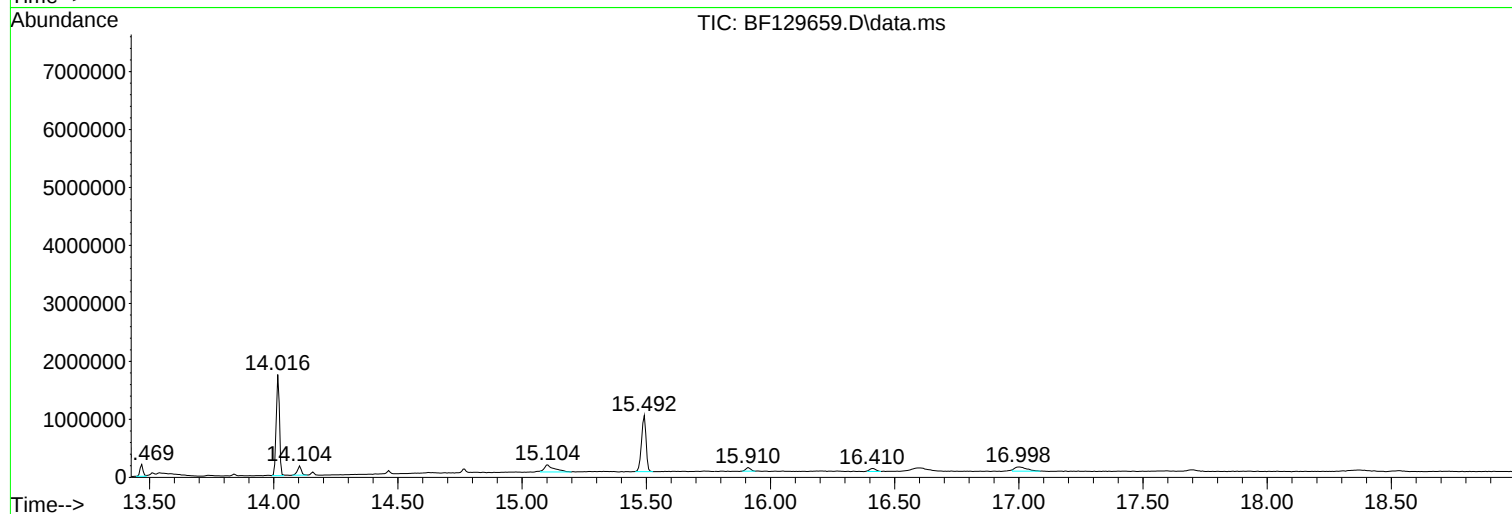
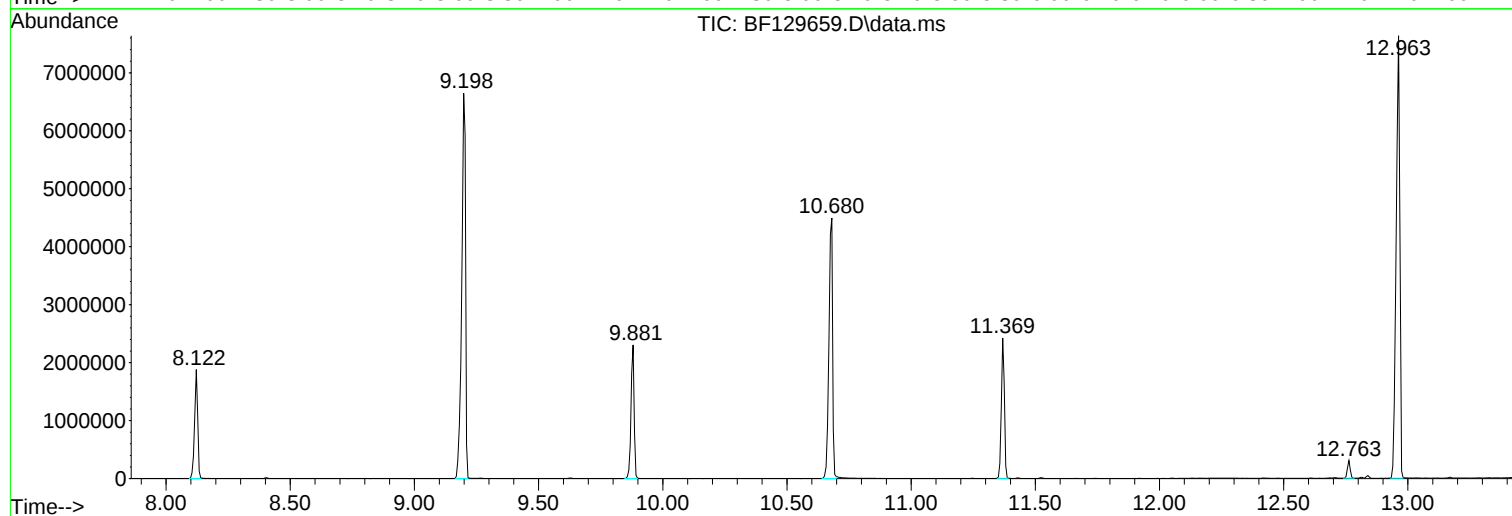
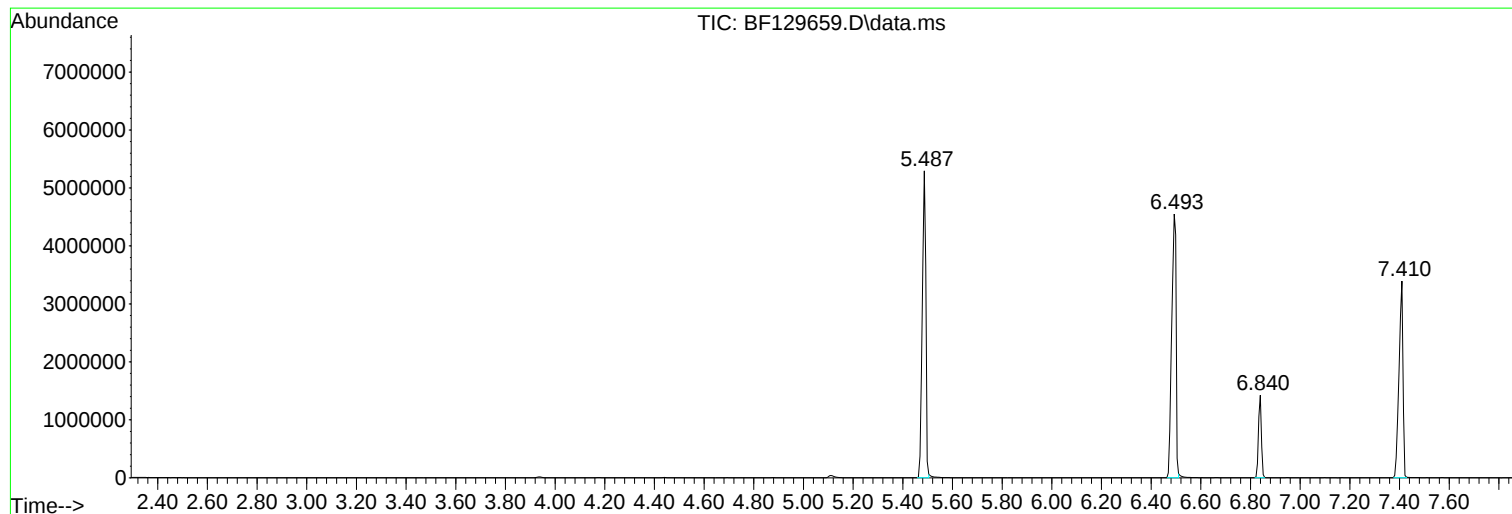
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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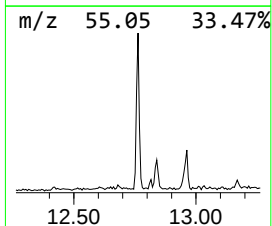
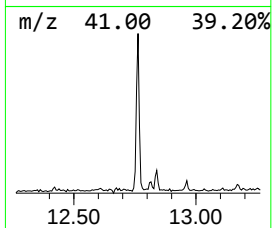
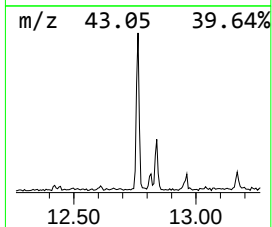
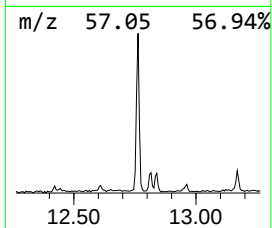
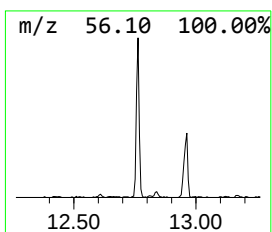
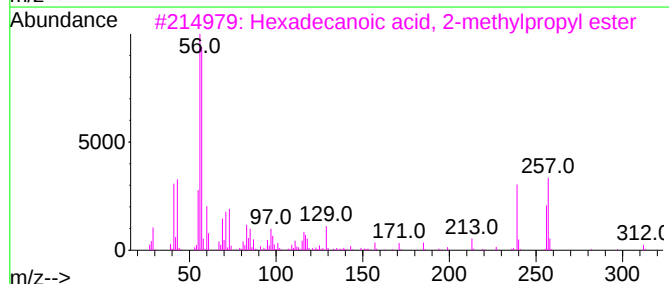
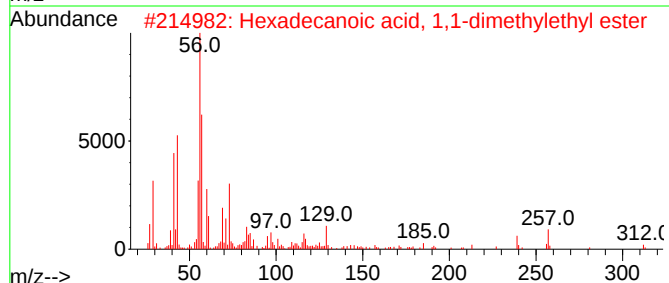
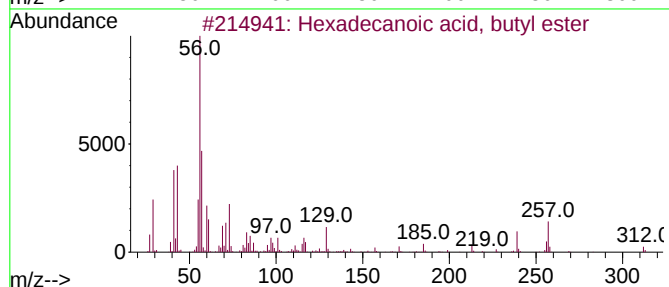
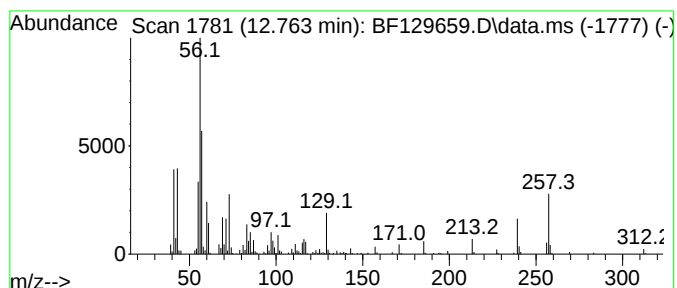
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.763	3.07 ng	237999	Chrysene-d12	14.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	99
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	70
4	1,3-Hexanediol, 2-ethyl- (isomer 1)	146	C8H18O2	1000484-18-2	37
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



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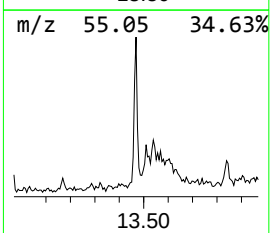
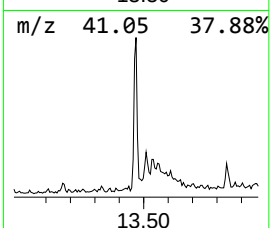
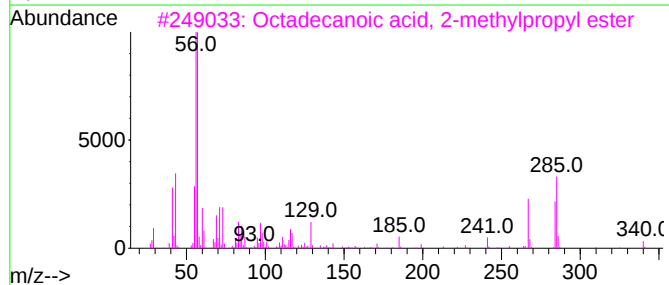
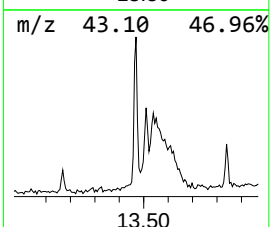
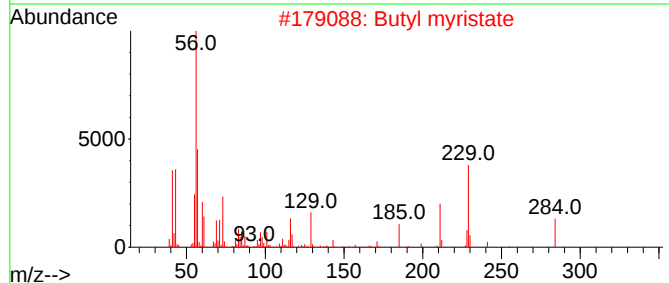
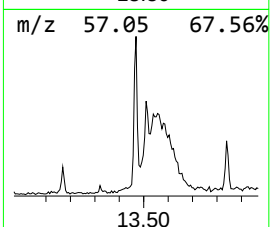
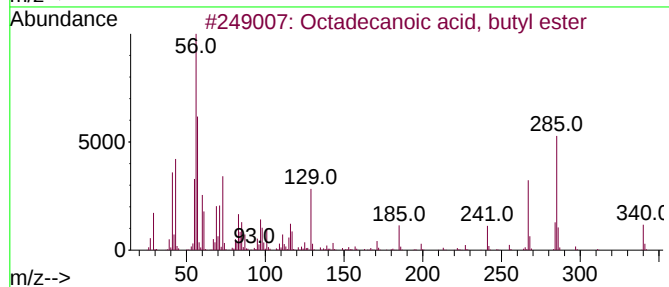
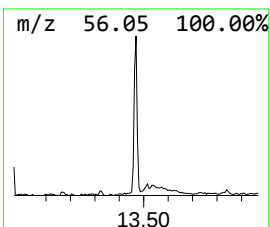
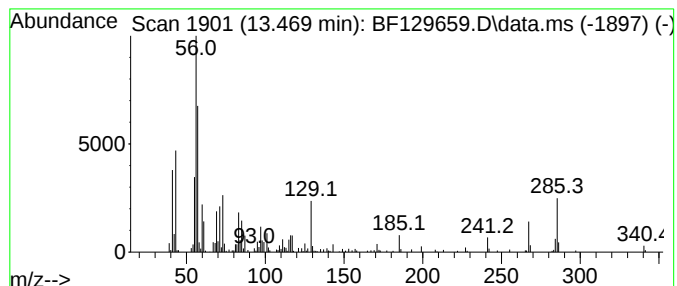
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.469	2.32 ng	180275	Chrysene-d12	14.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	97
2			Butyl myristate	284	C18H36O2	000110-36-1	72
3			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	70
4			Docosanoic acid, isobutyl ester	396	C26H52O2	1000405-17-1	47
5			Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	38



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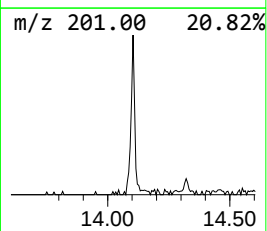
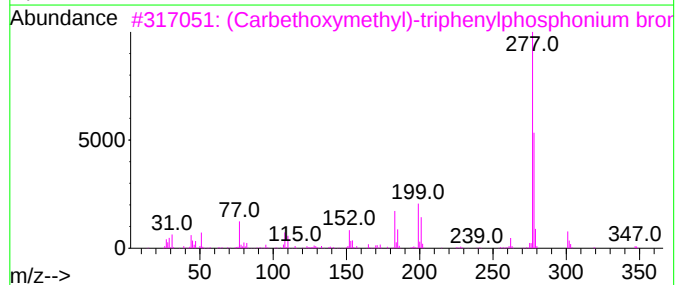
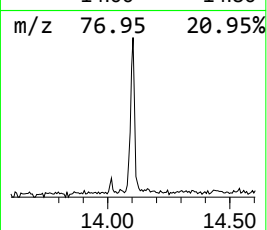
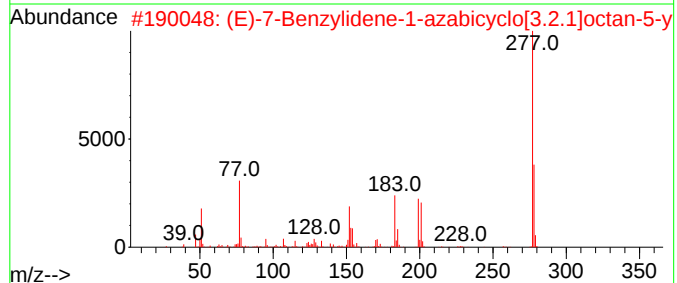
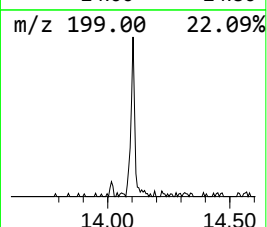
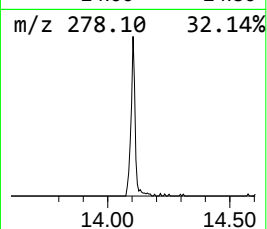
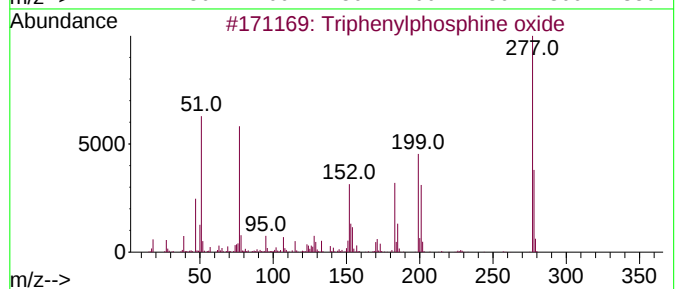
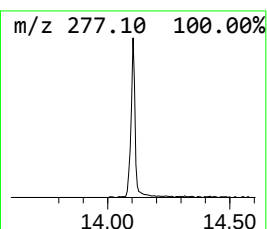
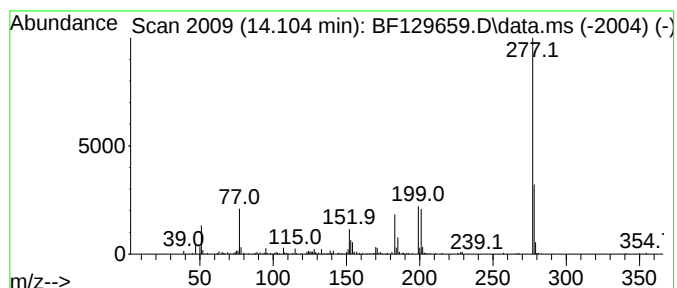
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.104	2.26 ng	174978	Chrysene-d12	14.016	
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	62
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	53
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	17



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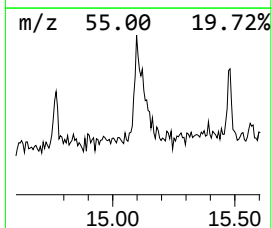
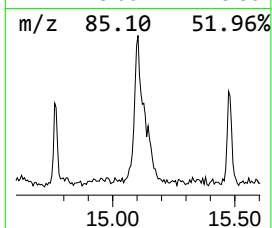
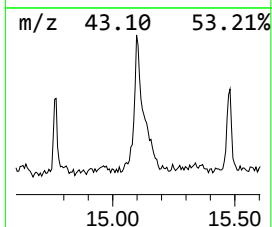
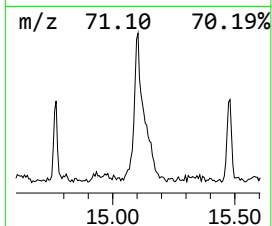
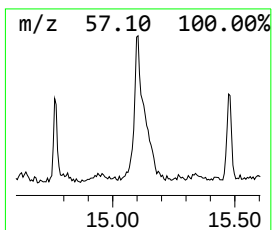
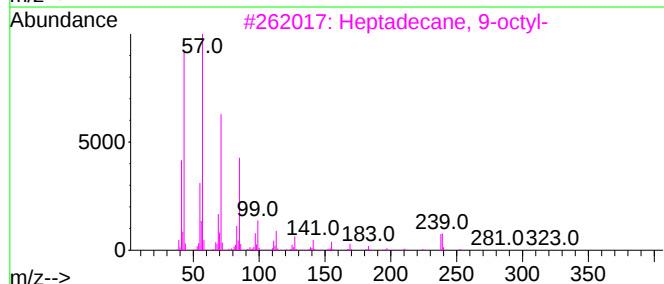
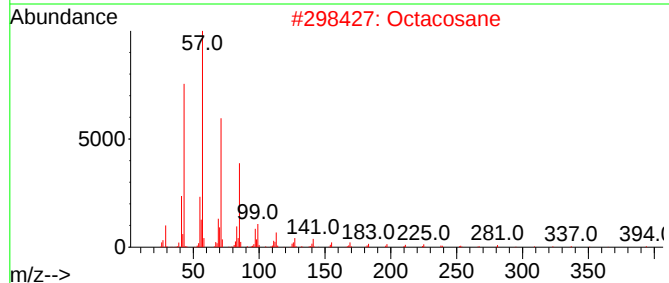
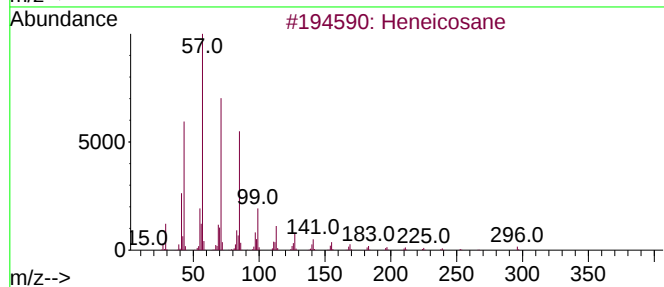
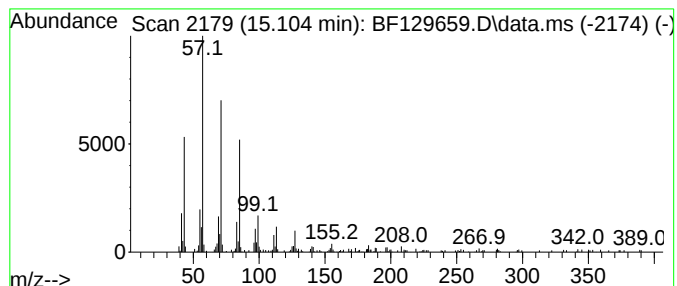
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Peak Number 4 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	5.37 ng	335699	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	94
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



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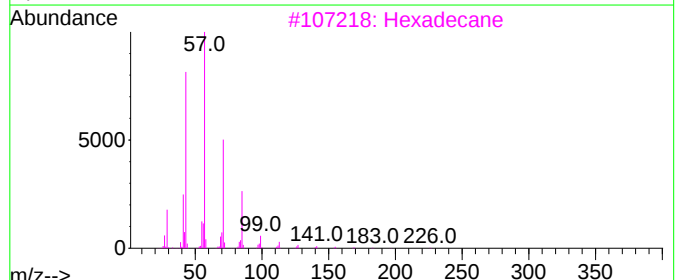
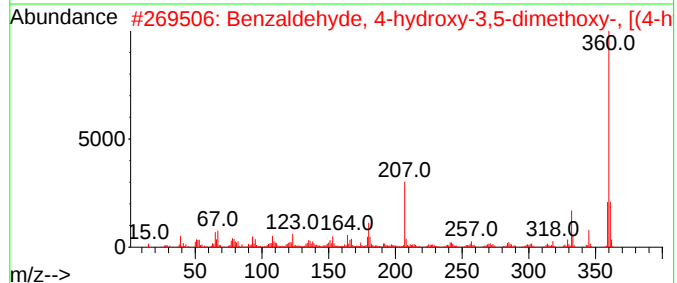
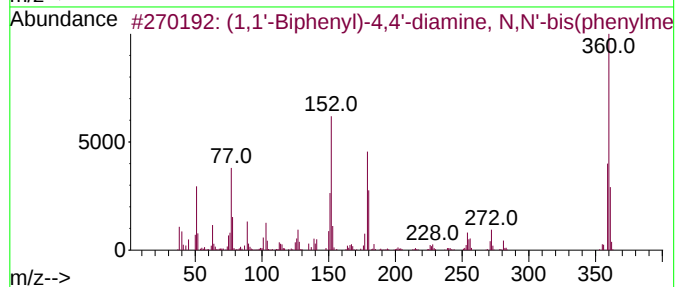
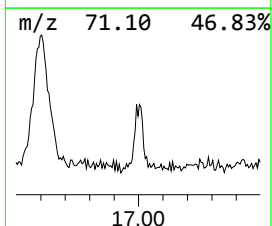
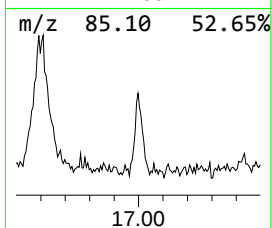
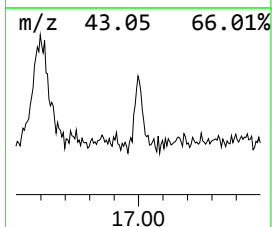
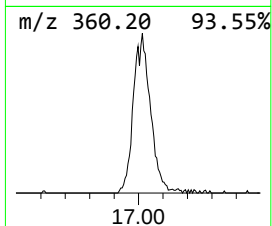
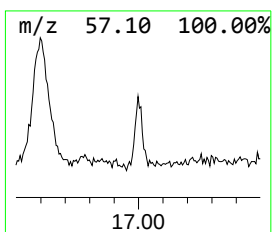
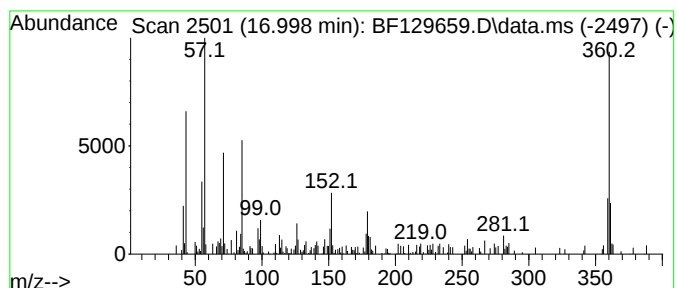
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Peak Number 5 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.998	3.93 ng	245631	Perylene-d12	15.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,N,N',N'-tetra-	360	C26H20N2	006311-48-4	78
2	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	360	C18H20N2O6	014414-32-5	43
3	Hexadecane	226	C16H34	000544-76-3	40
4	1,3,2-Dioxaborolane, bis(spiro[4.5]undec-5-en-2-ylidene)-	360	C20H13BO6	1000150-23-7	38
5	1H-isindole-1,3(2H)-dione, 2-[5-methyl-1H-indol-3-yl]-	360	C21H16N2O4	1000398-48-8	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	12.763	3.1	ng	237999	5	14.016	1550820	20.0
Octadecanoic ac...	13.469	2.3	ng	180275	5	14.016	1550820	20.0
Triphenylphosph...	14.104	2.3	ng	174978	5	14.016	1550820	20.0
Heneicosane	15.104	5.4	ng	335699	6	15.492	1249770	20.0
(1,1'-Biphenyl)...	16.998	3.9	ng	245631	6	15.492	1249770	20.0