

Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
 Data File : BG022964.D
 Acq On : 9 Jul 2016 14:05
 Operator : UM/SJ
 Sample : H3936-08
 Misc :
 ALS Vial : 59 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TW-4-DEP

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:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.613	293	302	315	rBV	1251550	1925858	18.56%	4.159%
2	5.224	399	406	420	rBV	1297328	2018656	19.46%	4.360%
3	5.694	479	486	494	rBV	530867	898219	8.66%	1.940%
4	6.311	585	591	597	rVB	266512	416048	4.01%	0.899%
5	7.304	754	760	769	rVB	406045	713894	6.88%	1.542%
6	7.680	817	824	833	rBV	1065288	1858679	17.92%	4.014%
7	8.150	896	904	911	rBV	370815	649749	6.26%	1.403%
8	8.479	952	960	968	rBV	1424727	2440725	23.53%	5.271%
9	9.325	1095	1104	1114	rBV	1383472	2483330	23.94%	5.363%
10	10.976	1378	1385	1394	rVB	555457	1018566	9.82%	2.200%
11	13.415	1791	1800	1808	rBV	4192249	6541316	63.06%	14.127%
12	14.237	1934	1940	1945	rBV	111591	175310	1.69%	0.379%
13	14.795	2028	2035	2044	rBV2	1006705	1711375	16.50%	3.696%
14	16.288	2281	2289	2305	rBV	2806452	4202481	40.51%	9.076%
15	17.551	2496	2504	2517	rBV2	1357616	2208939	21.29%	4.771%
16	18.420	2646	2652	2658	rBV2	207572	285184	2.75%	0.616%
17	19.684	2864	2867	2876	rVB3	130060	170295	1.64%	0.368%
18	19.825	2886	2891	2897	rBV	1019070	1236191	11.92%	2.670%
19	20.154	2941	2947	2957	rBV	7788879	10373954	100.00%	22.404%
20	21.846	3229	3235	3243	rVB2	1495784	2536369	24.45%	5.478%
21	25.207	3796	3807	3818	rVB2	797766	2438009	23.50%	5.265%

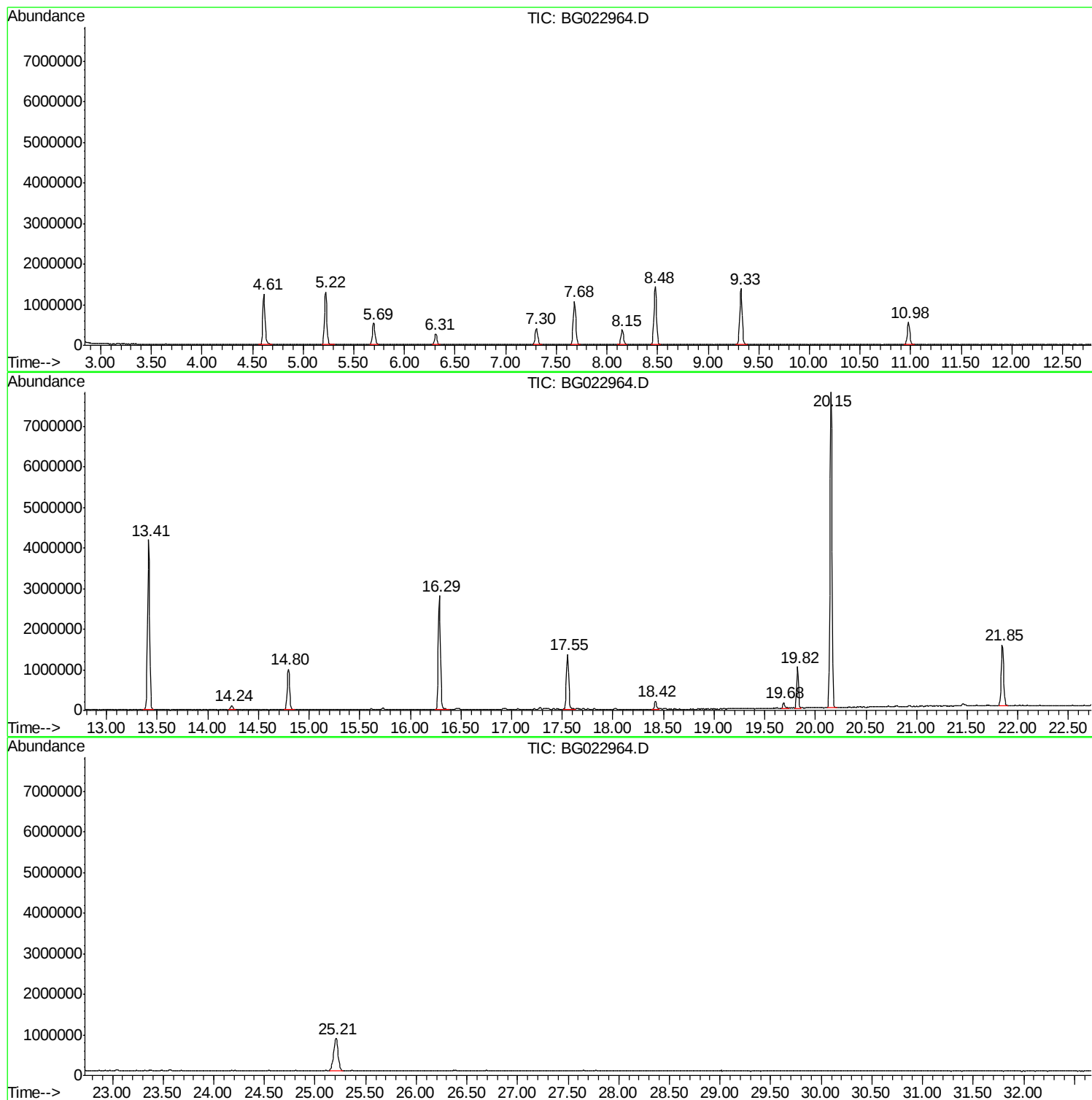
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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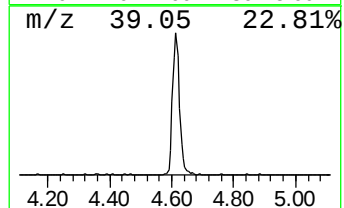
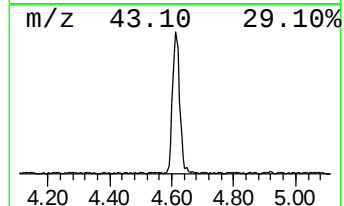
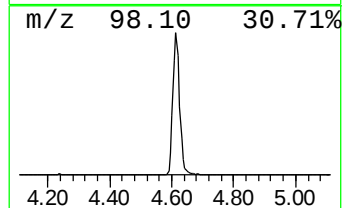
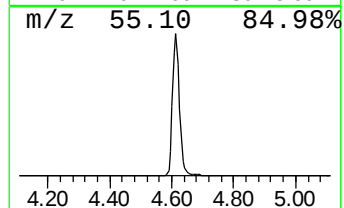
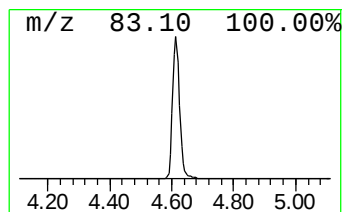
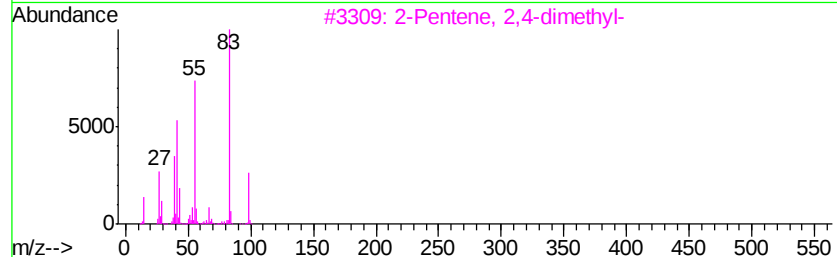
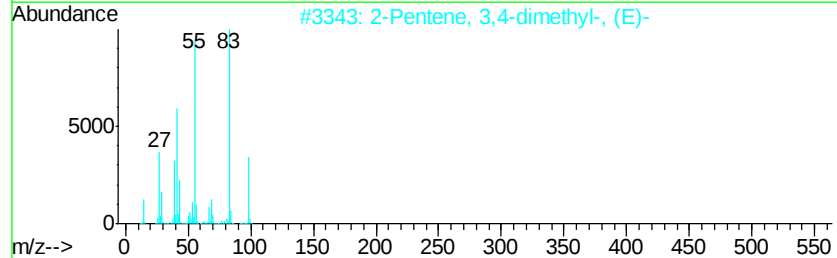
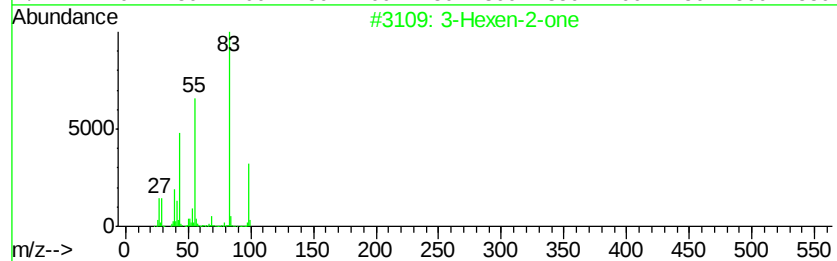
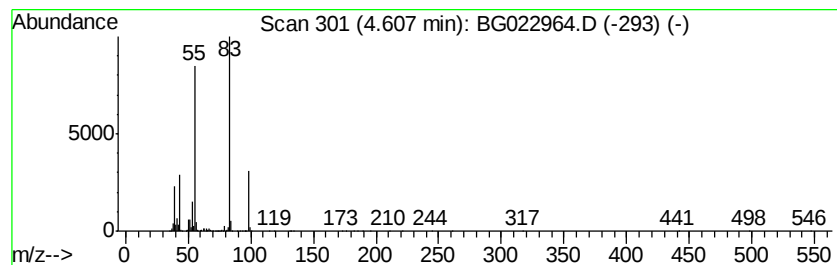
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	59.28 ng	1925860	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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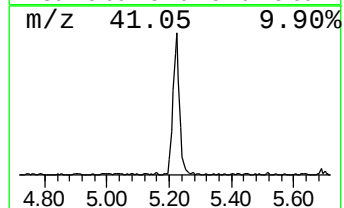
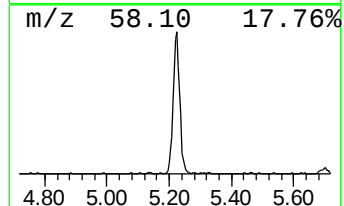
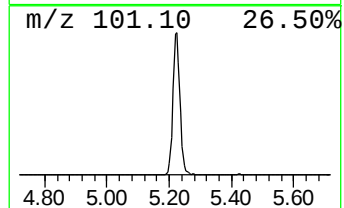
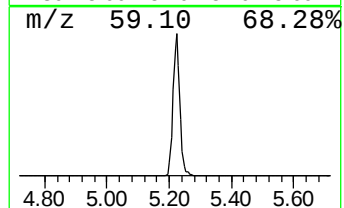
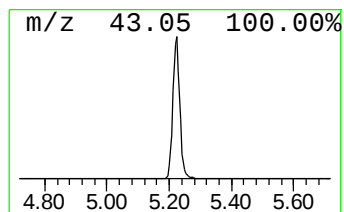
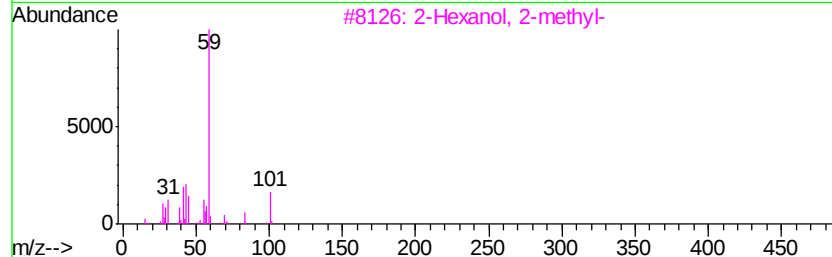
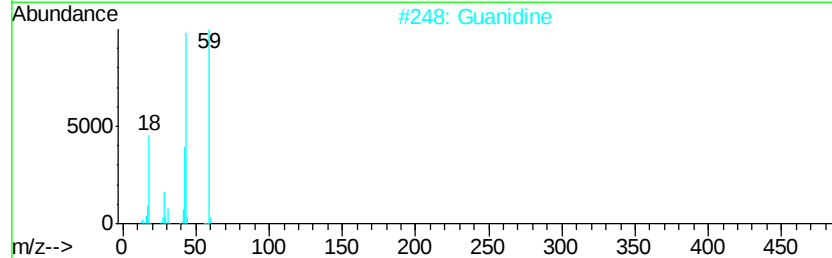
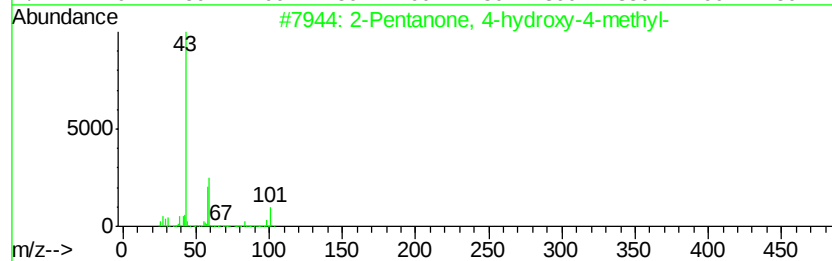
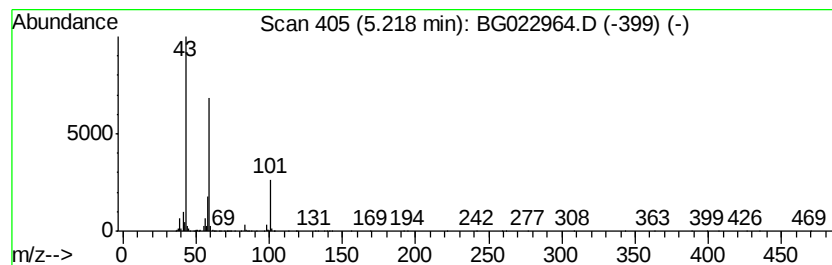
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	62.14 ng	2018660	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	43
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25



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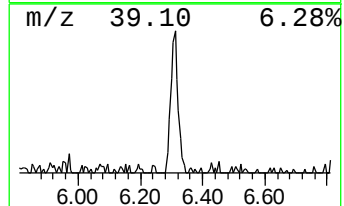
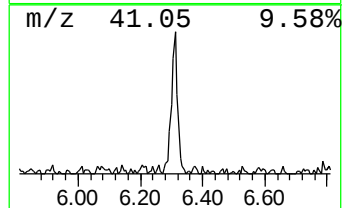
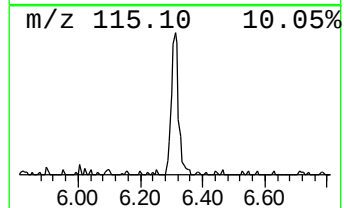
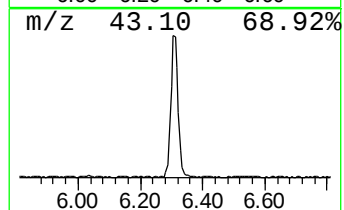
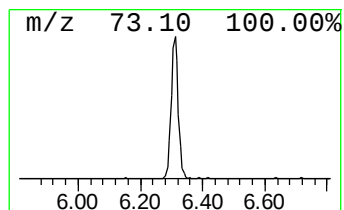
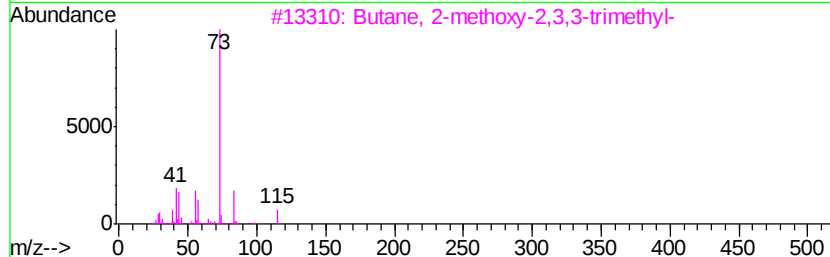
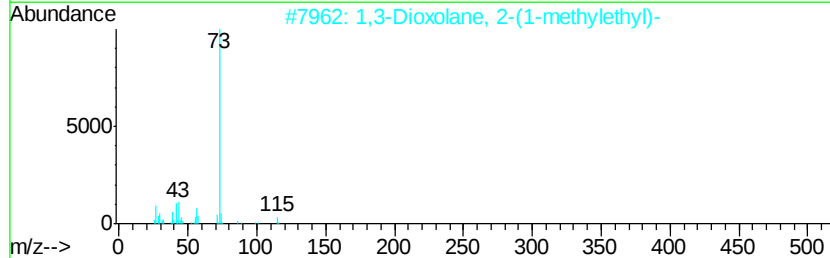
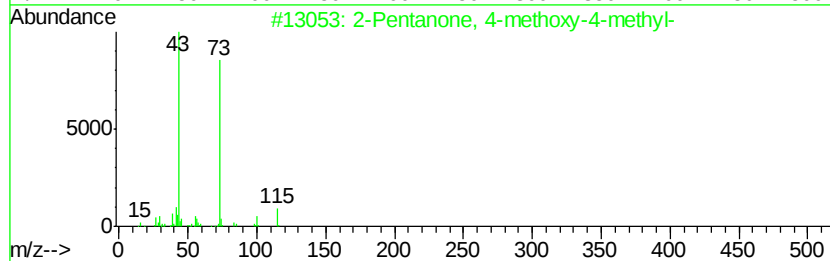
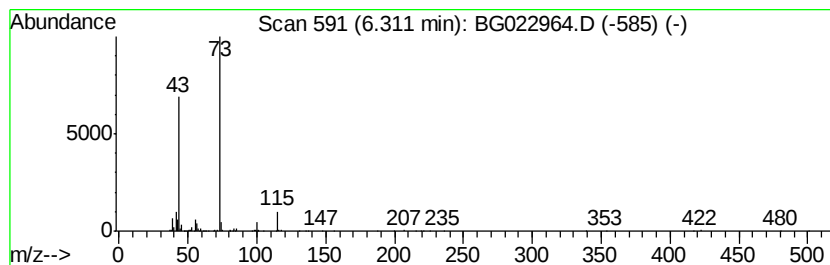
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.31	12.81 ng	416048	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	59
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	37
3		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	36
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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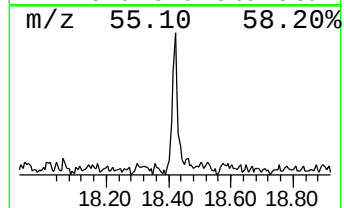
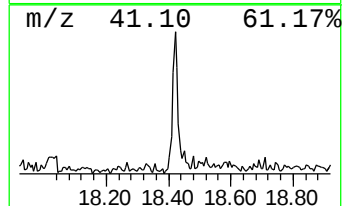
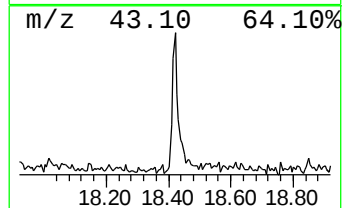
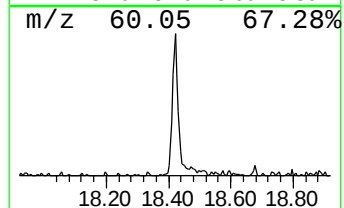
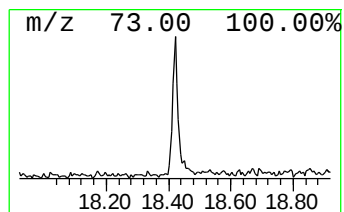
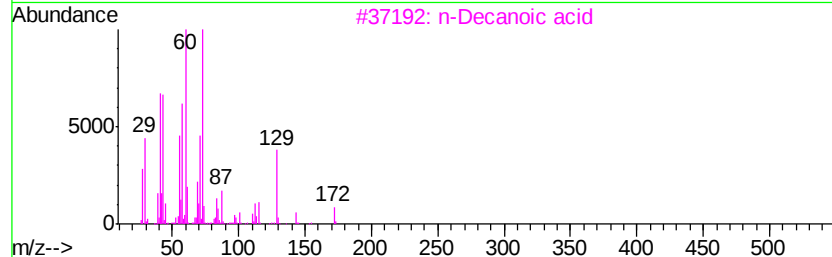
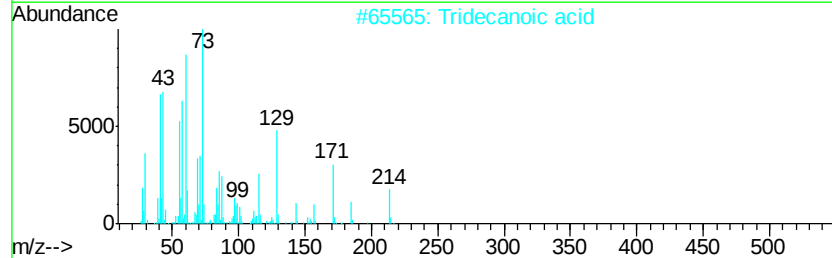
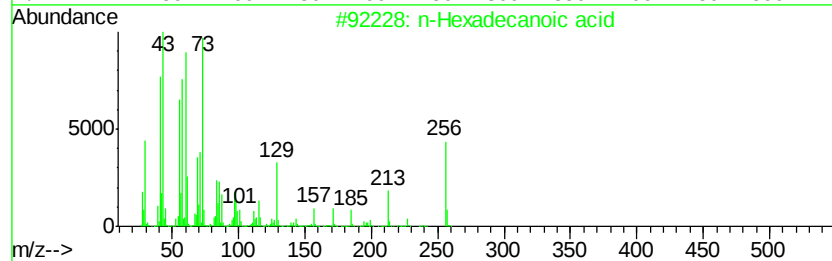
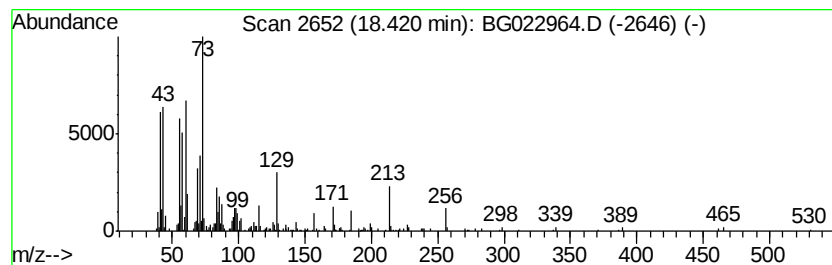
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.58 ng	285184	Phenanthrene-d10	17.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	55
3		n-Decanoic acid	172	C10H20O2	000334-48-5	53
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5		Nonadecanoic acid	298	C19H38O2	000646-30-0	38



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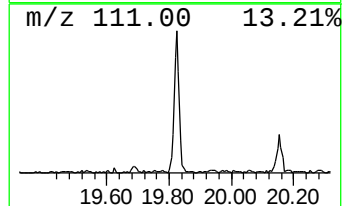
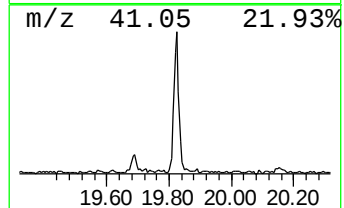
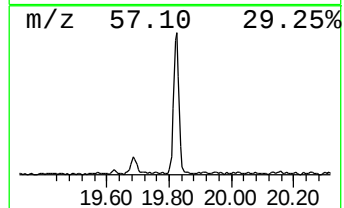
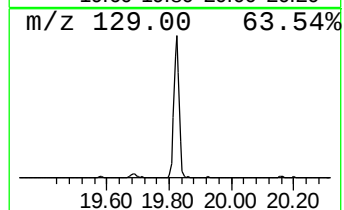
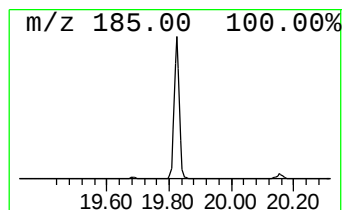
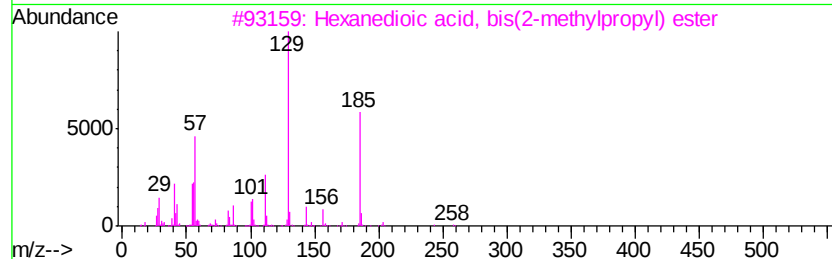
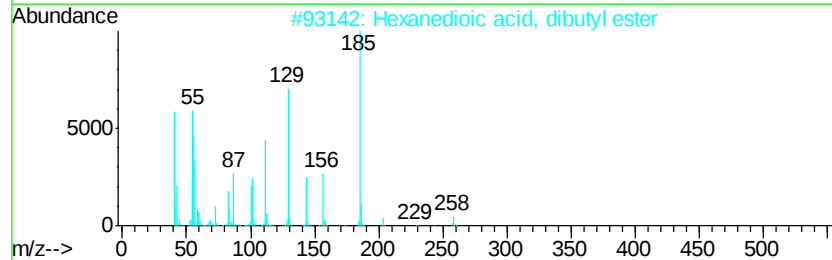
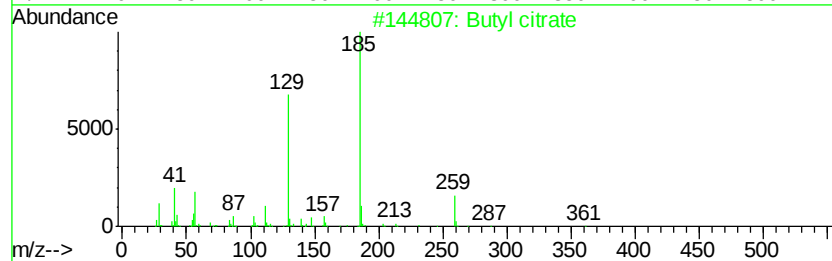
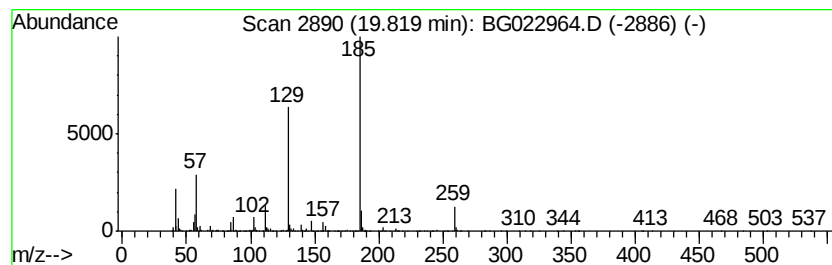
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Peak Number 7 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.82	9.75 ng	1236190	Chrysene-d12	21.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butyl citrate	360	C18H32O7	000077-94-1	91
2		Hexanedioic acid, dibutyl ester	258	C14H26O4	000105-99-7	50
3		Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	50
4		Indole, 3-(1,3,4-oxadiazol-2-yl)-	185	C10H7N3O	082380-80-1	28
5		Hexanedioic acid, bis(1-methylpr...	258	C14H26O4	038447-22-2	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.61	59.3	ng	1925860	1	8.15	649749	20.0
2-Pentanone, 4-hy...	5.22	62.1	ng	2018660	1	8.15	649749	20.0
2-Pentanone, 4-me...	6.31	12.8	ng	416048	1	8.15	649749	20.0
n-Hexadecanoic acid	18.42	2.6	ng	285184	4	17.55	2208940	20.0
Butyl citrate	19.82	9.8	ng	1236190	5	21.85	2536370	20.0