

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
 Data File : BF124049.D
 Acq On : 25 May 2021 17:18
 Operator : JU/CG
 Sample : PB136628BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136628BL

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-BF051421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	27	34	40	rVB	81826	117303	3.46%	0.634%
2	5.140	513	519	528	rVB	608101	821711	24.23%	4.440%
3	5.534	580	586	589	rBV	2212398	2240150	66.06%	12.105%
4	5.916	647	651	655	rBB	70224	64129	1.89%	0.347%
5	6.528	748	755	757	rBV	1932573	2212645	65.25%	11.956%
6	6.892	813	817	821	rBV	534695	402314	11.86%	2.174%
7	7.457	907	913	916	rBV	1492787	1556902	45.91%	8.413%
8	8.175	1030	1035	1039	rBV	559076	505172	14.90%	2.730%
9	9.257	1212	1219	1222	rBV	2969528	2821607	83.20%	15.247%
10	9.933	1329	1334	1337	rBV	789824	607617	17.92%	3.283%
11	10.727	1463	1469	1472	rBV	2245170	2006574	59.17%	10.843%
12	11.422	1583	1587	1591	rBV	771694	642583	18.95%	3.472%
13	13.016	1852	1858	1861	rBV	3384722	3391253	100.00%	18.325%
14	13.857	1995	2001	2004	rBV3	23955	36296	1.07%	0.196%
15	13.933	2011	2014	2019	rVB	72374	67992	2.00%	0.367%
16	14.068	2033	2037	2040	rVB	661428	541326	15.96%	2.925%
17	15.562	2286	2291	2302	rBV	339885	470383	13.87%	2.542%

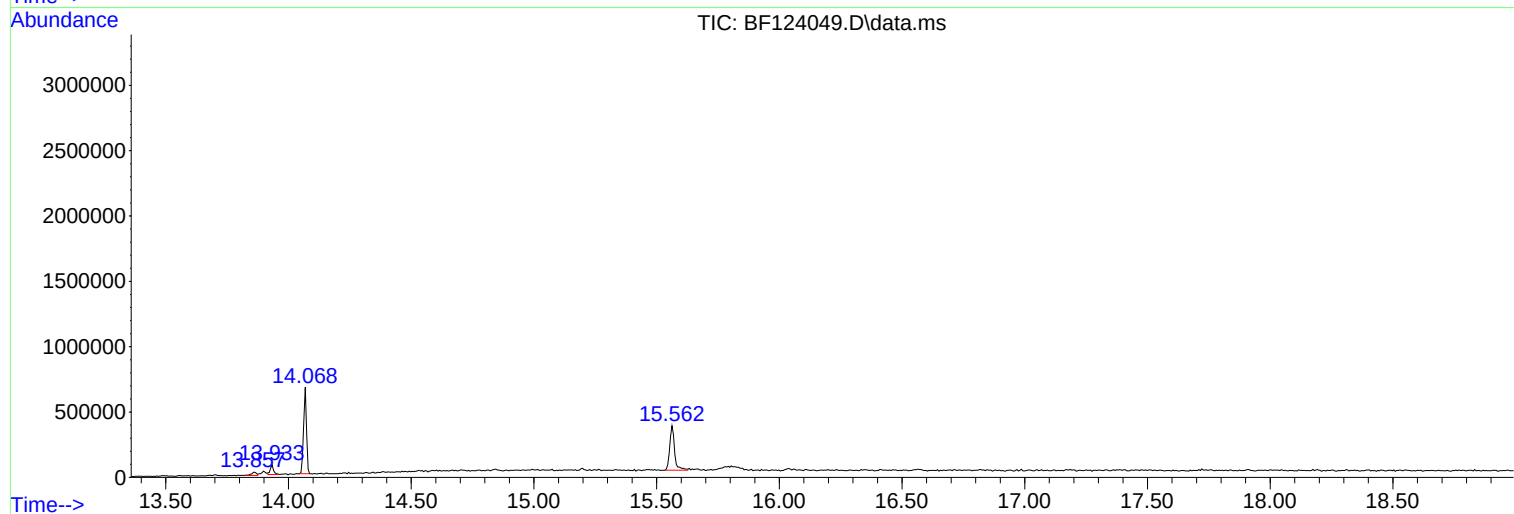
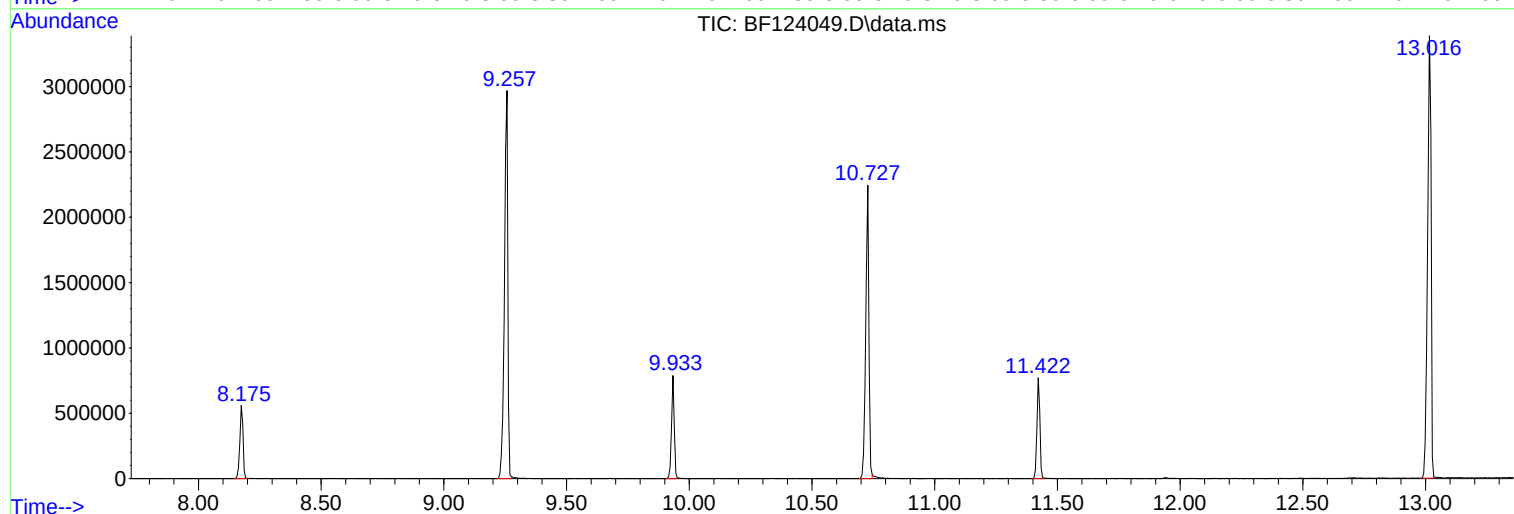
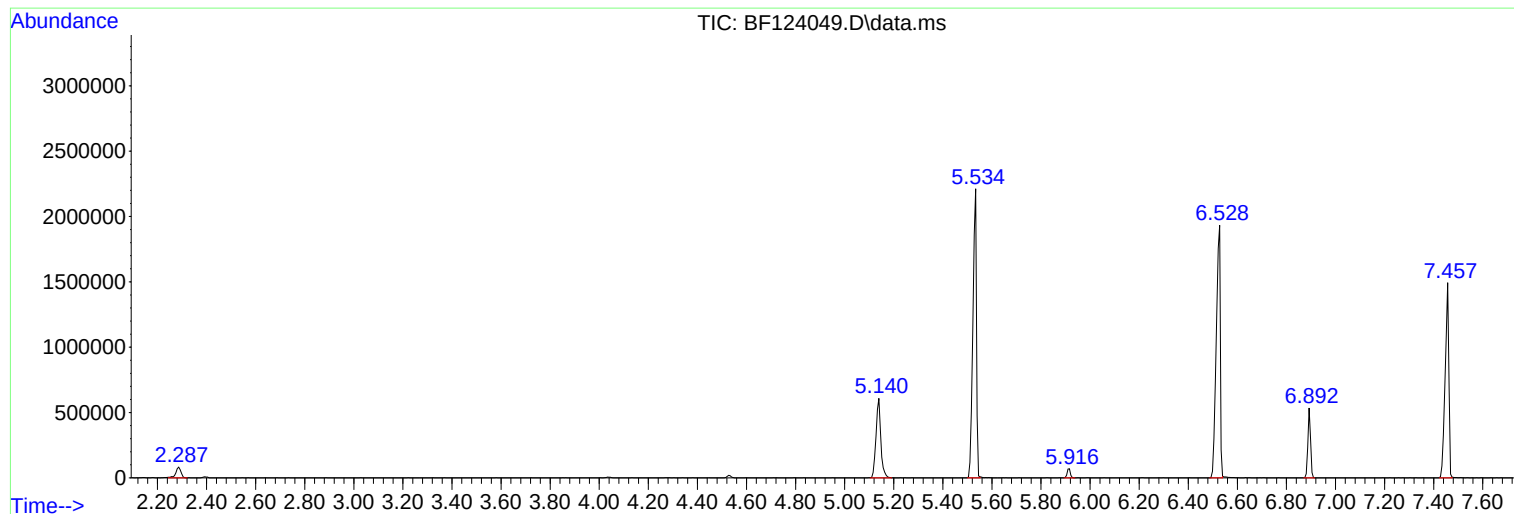
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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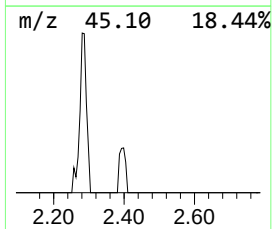
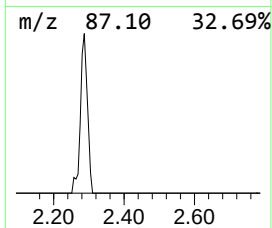
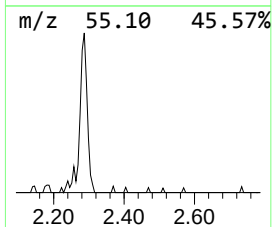
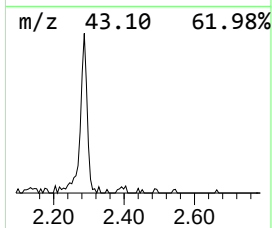
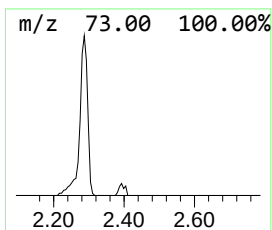
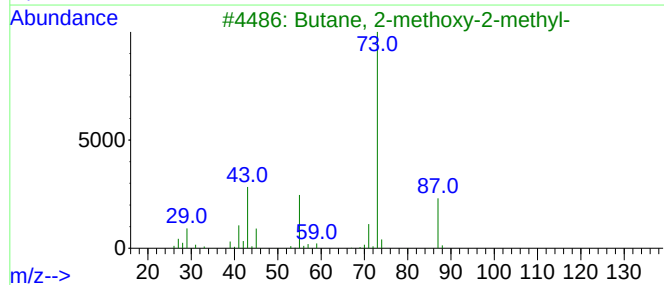
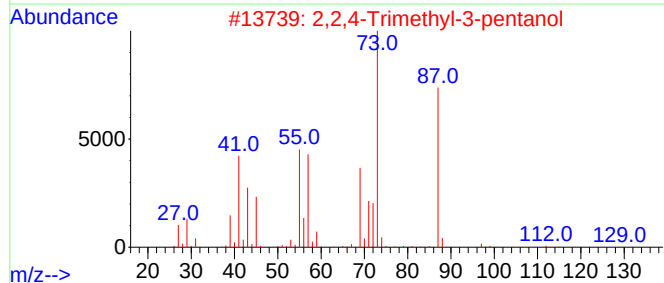
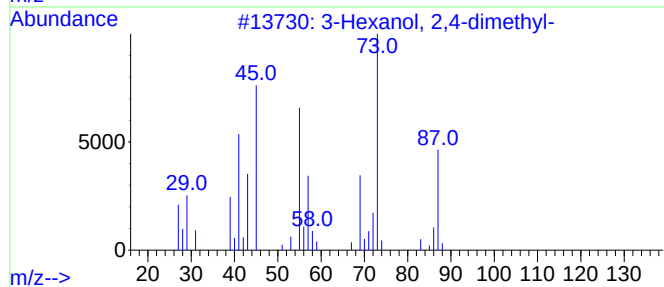
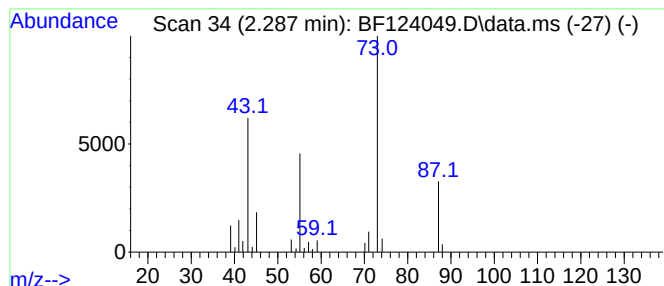
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.28 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	5.83 ng	117303	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	45
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	37
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	10



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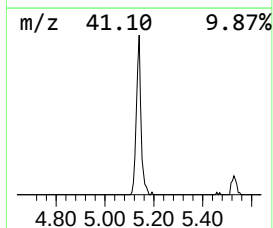
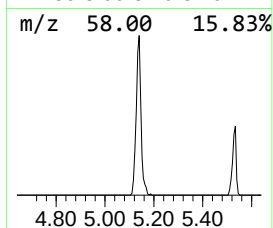
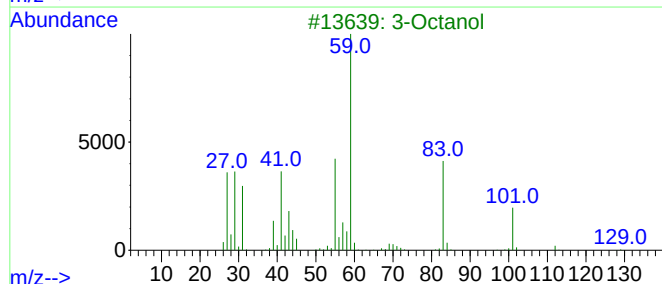
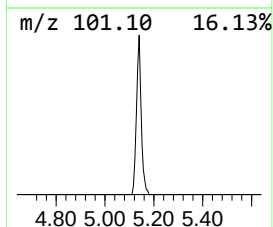
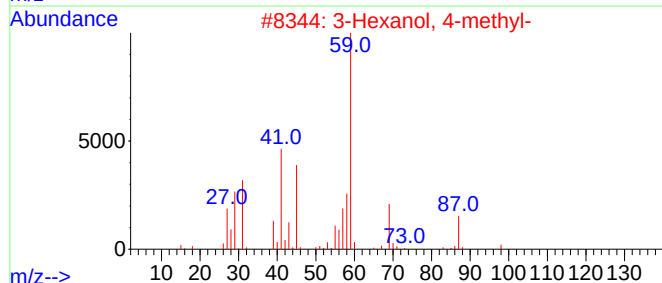
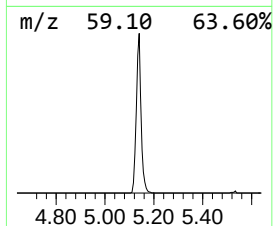
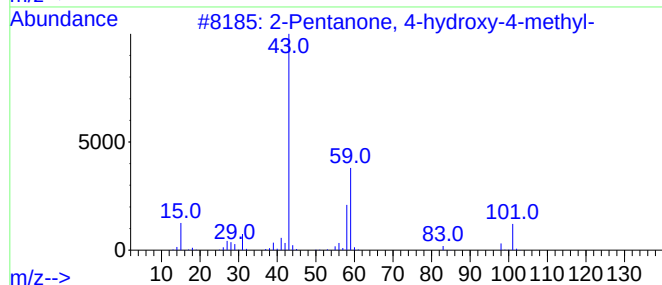
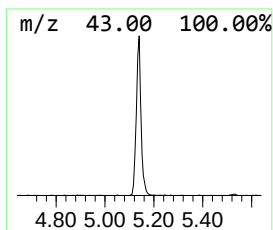
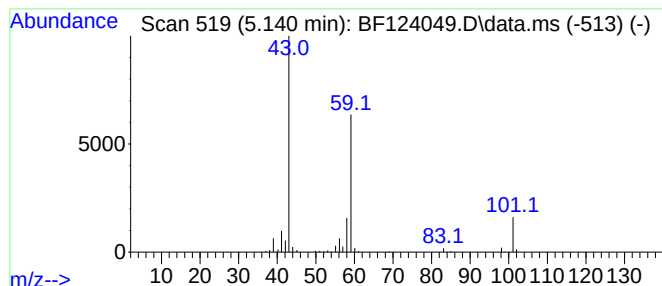
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	40.85 ng	821711	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			3-Octanol	130	C8H18O	000589-98-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28



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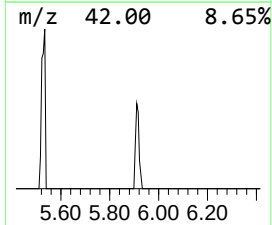
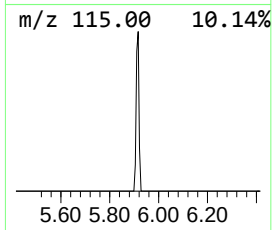
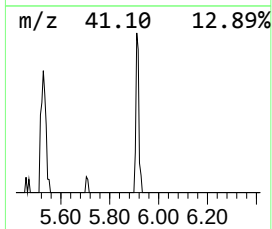
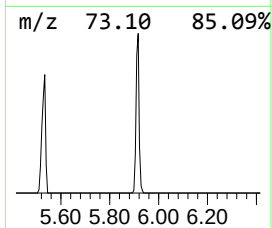
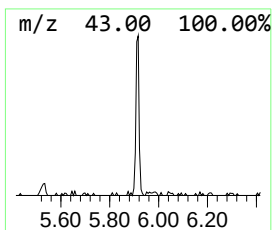
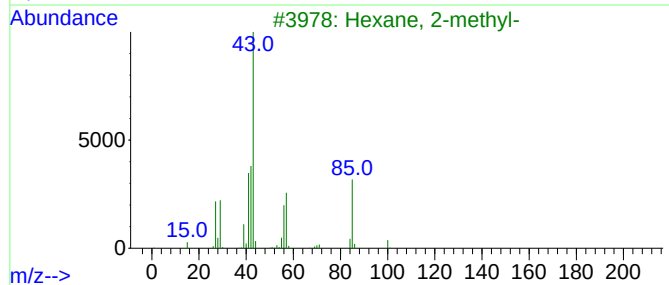
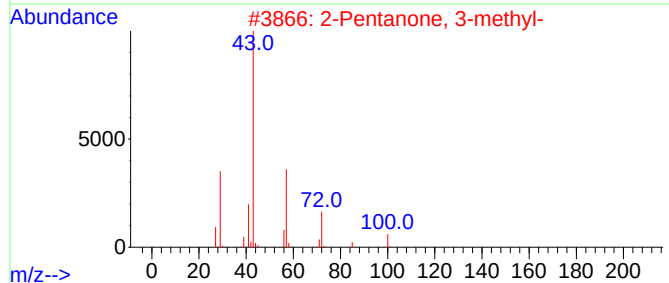
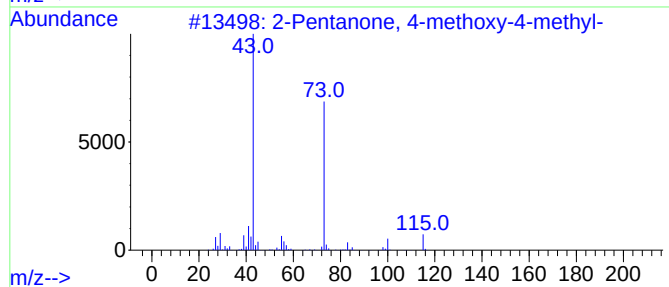
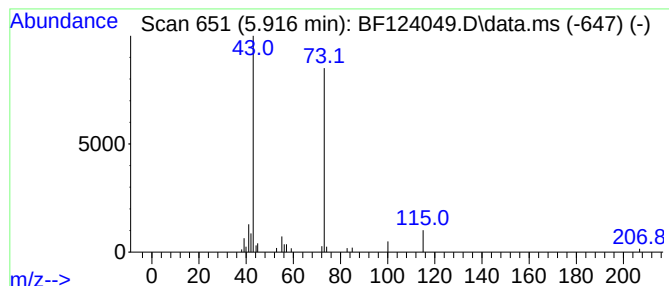
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.916	3.19 ng	64129	1,4-Dichlorobenzene-d4	6.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
3		Hexane, 2-methyl-	100	C7H16	000591-76-4	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



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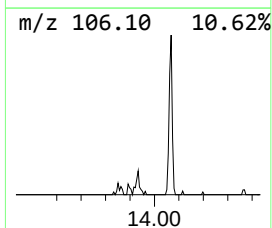
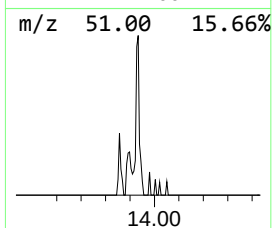
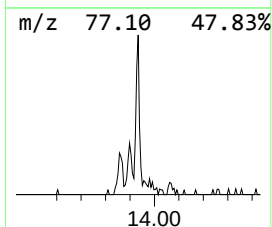
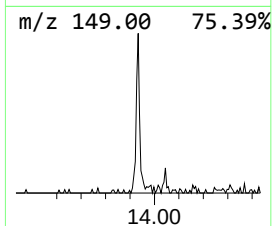
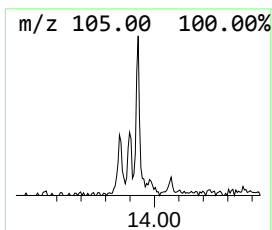
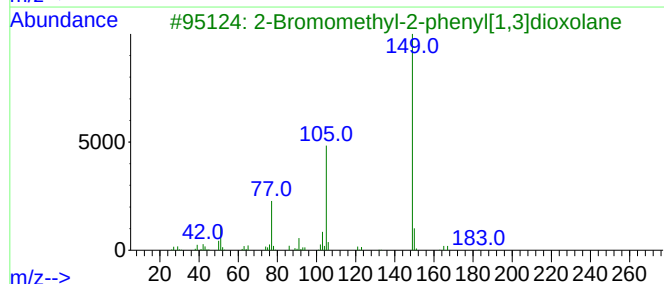
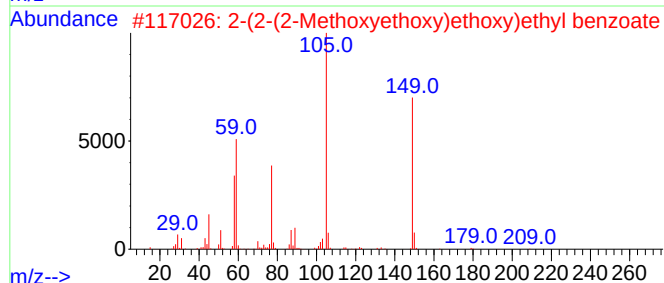
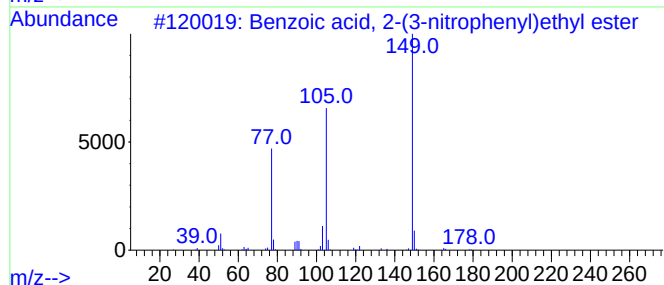
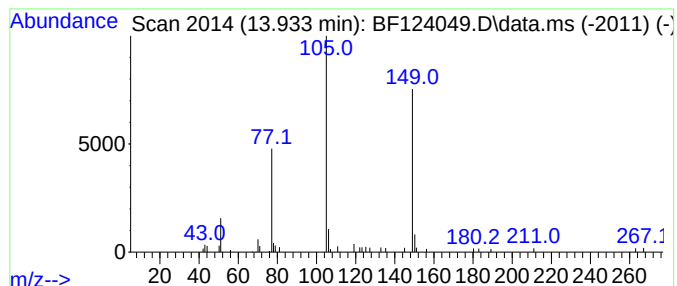
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Peak Number 4 Benzoic acid, 2-(3-nitrophe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	2.51 ng	67992	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
2			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	78
3			2-Bromomethyl-2-phenyl[1,3]dioxo...	242	C10H11BrO2	003418-21-1	78
4			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
5			2-(2-(2-Ethoxyethoxy)ethoxy)ethy...	282	C15H22O5	1000366-98-8	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.28	2.287	5.8	ng	117303	1	6.892	402314	20.0
2-Pentanone, 4-...	5.140	40.9	ng	821711	1	6.892	402314	20.0
2-Pentanone, 4-...	5.916	3.2	ng	64129	1	6.892	402314	20.0
Benzoic acid, 2...	13.933	2.5	ng	67992	5	14.069	541326	20.0