

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
 Data File : BF126252.D
 Acq On : 18 Dec 2021 14:05
 Operator : JU/CG
 Sample : M5168-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-08-C

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126252.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	11	rVB	87551	104484	3.01%	0.341%
2	2.222	17	23	29	rVB	62362	80550	2.32%	0.263%
3	4.404	390	394	401	rVB	42534	49056	1.42%	0.160%
4	5.028	494	500	512	rVB	1309510	1593553	45.97%	5.198%
5	5.428	563	568	571	rBV	3585785	3343366	96.45%	10.906%
6	5.828	633	636	640	rVB	205255	166442	4.80%	0.543%
7	6.439	734	740	743	rBV	3354415	3457241	99.74%	11.277%
8	6.816	800	804	807	rBV	1574336	1319349	38.06%	4.304%
9	7.375	894	899	902	rBV	2485203	2274866	65.63%	7.420%
10	8.098	1017	1022	1025	rBV	2078819	1850569	53.39%	6.036%
11	9.175	1200	1205	1208	rBV	3804516	3466362	100.00%	11.307%
12	9.263	1216	1220	1224	rVB2	52211	50112	1.45%	0.163%
13	9.851	1315	1320	1330	rBV	2232282	1996817	57.61%	6.513%
14	10.639	1449	1454	1457	rBV	2281778	2129778	61.44%	6.947%
15	11.304	1562	1567	1569	rBV3	43504	53766	1.55%	0.175%
16	11.333	1569	1572	1576	rVV	2030055	1954495	56.38%	6.375%
17	11.863	1659	1662	1666	rBV	48370	44001	1.27%	0.144%
18	12.139	1703	1709	1712	rBV6	33385	54981	1.59%	0.179%
19	12.921	1838	1842	1846	rBV	3171463	3214340	92.73%	10.485%
20	13.404	1914	1924	1929	rBV9	18215	42496	1.23%	0.139%
21	13.857	1994	2001	2012	rBV2	148785	412445	11.90%	1.345%
22	13.974	2016	2021	2024	rBV	1619735	1574578	45.42%	5.136%
23	14.068	2032	2037	2043	rVB	91278	102962	2.97%	0.336%
24	15.421	2261	2267	2273	rBV	999046	1320179	38.09%	4.306%

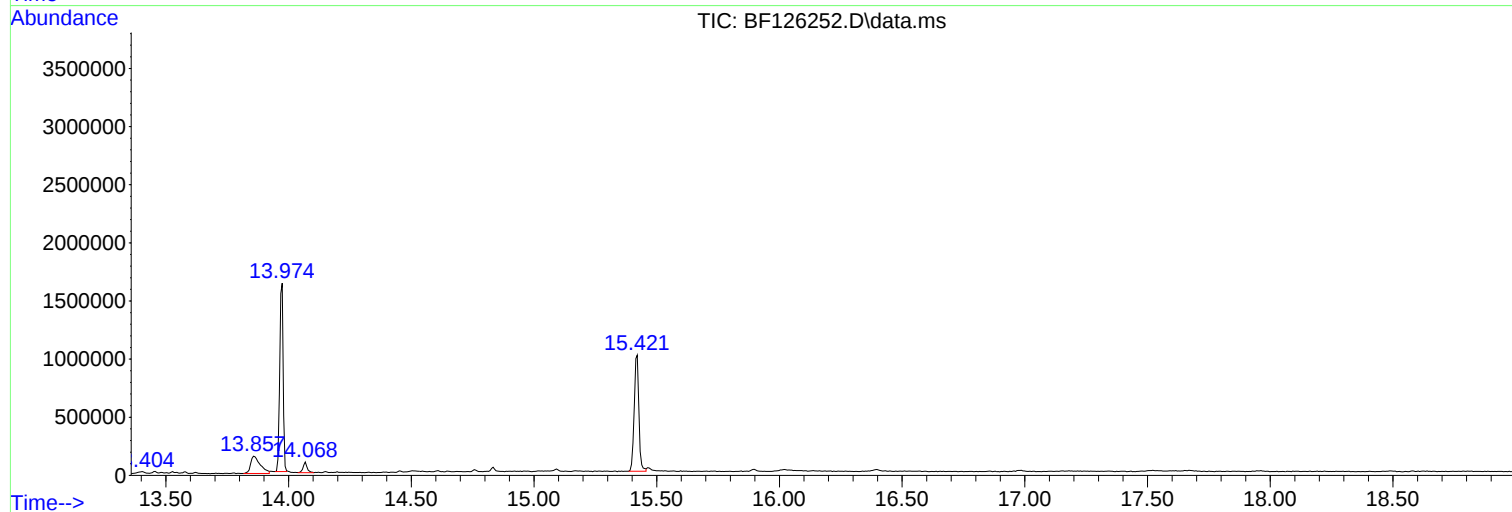
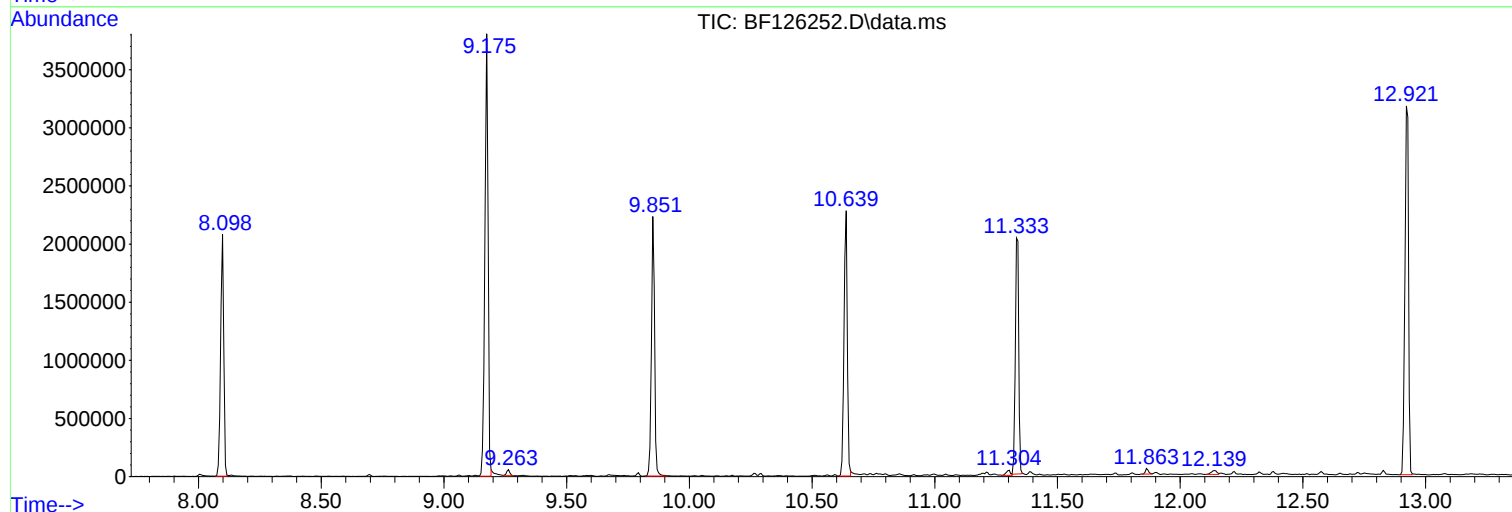
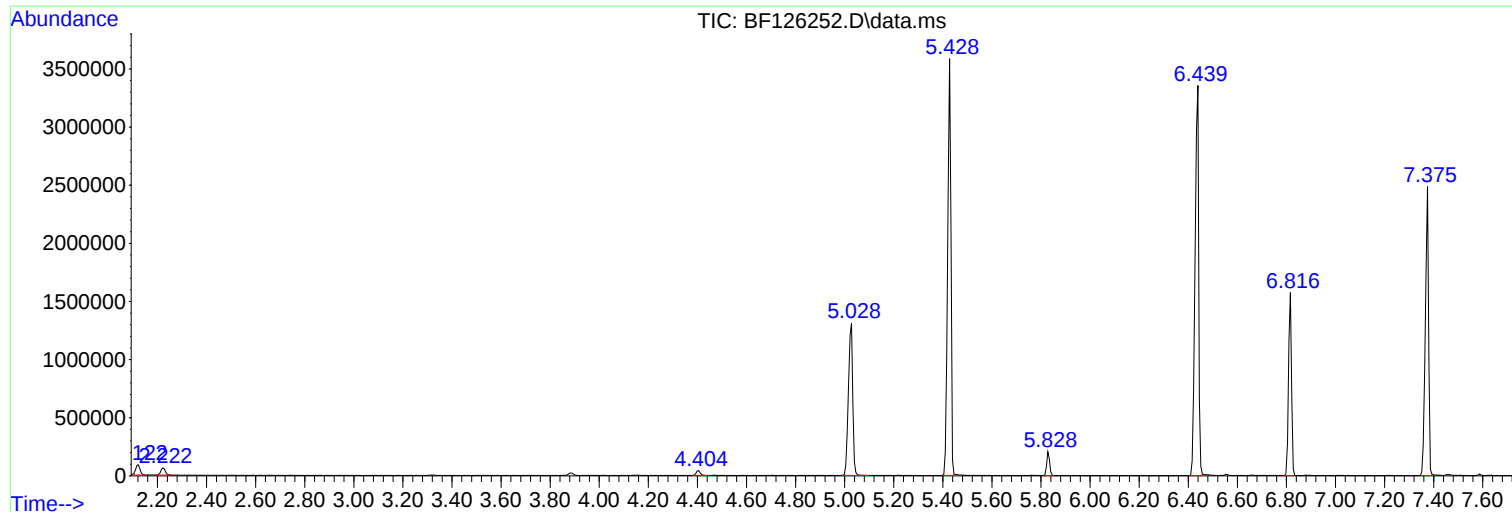
Sum of corrected areas: 30656788

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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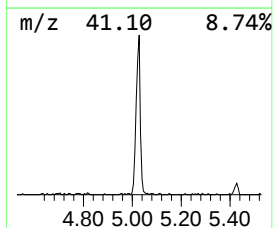
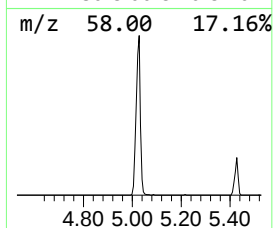
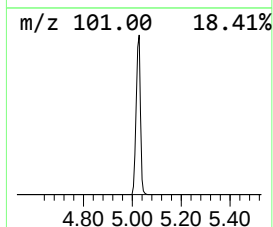
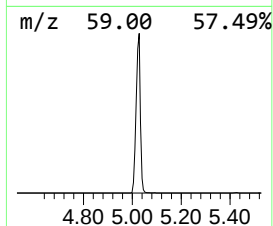
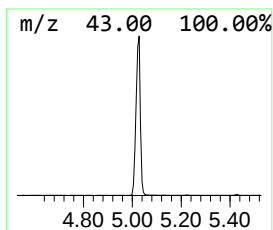
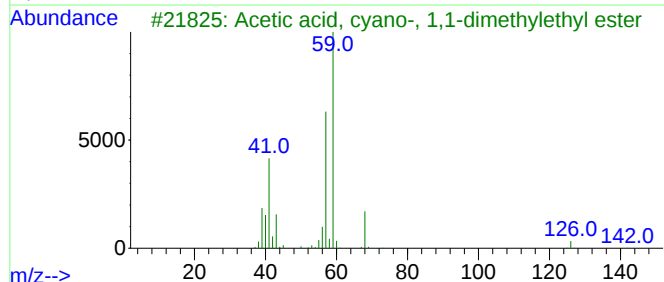
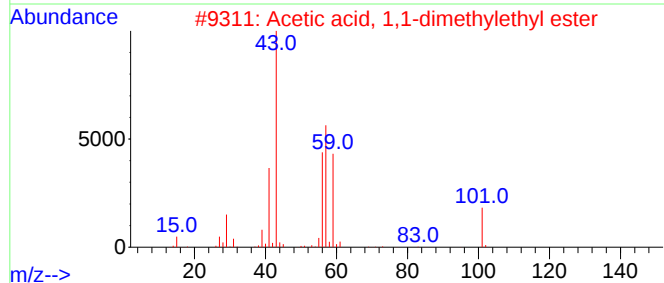
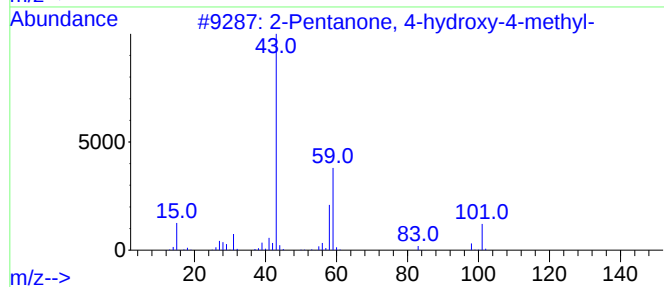
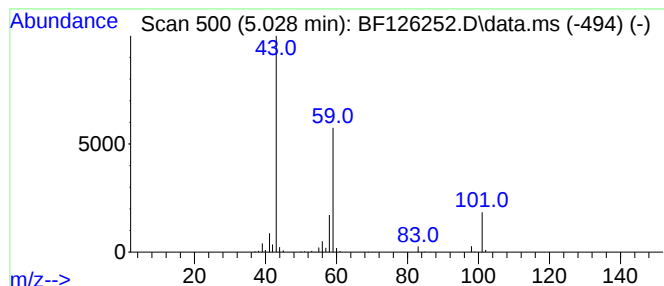
Instrument :
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ClientSampleId :
SB-08-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
5.028	24.16 ng	1593550	1,4-Dichlorobenzene-d4	6.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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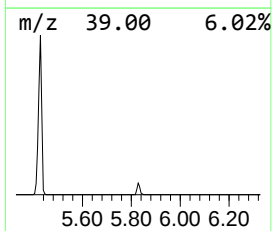
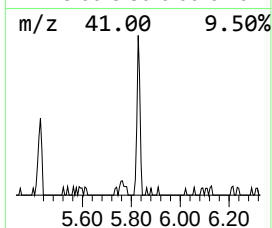
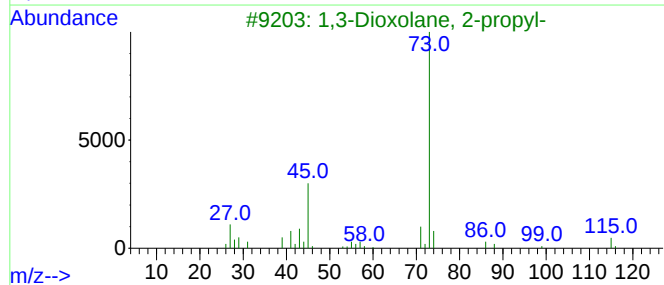
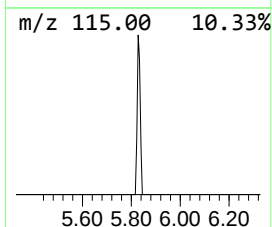
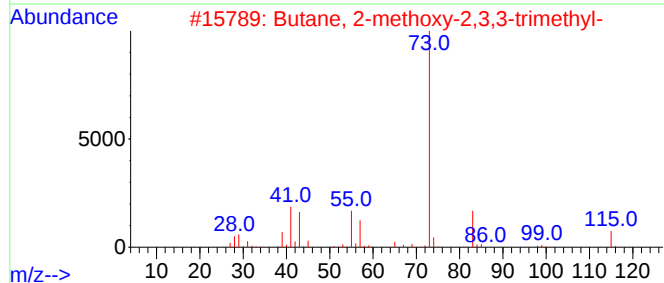
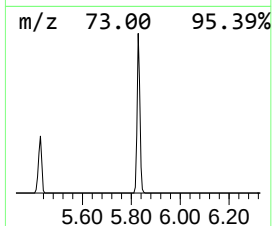
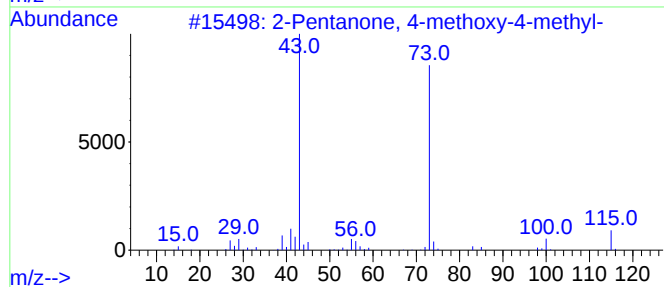
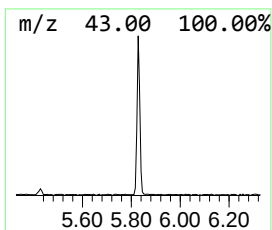
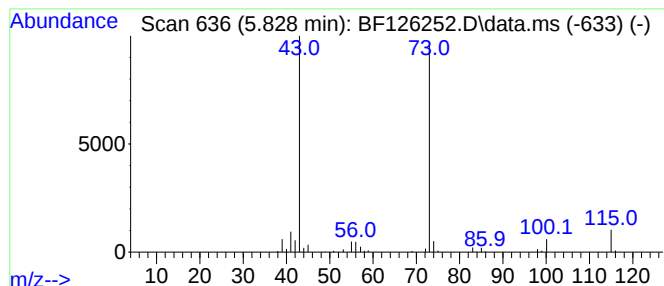
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	2.52 ng	166442	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10



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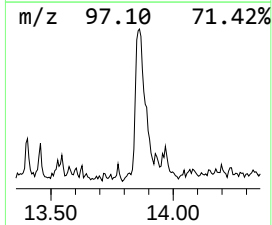
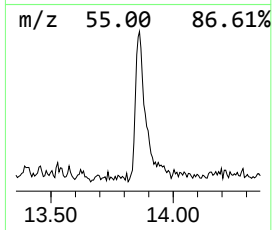
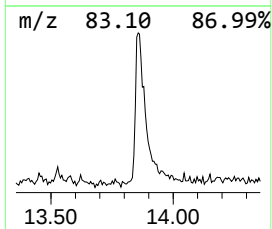
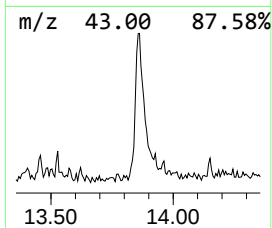
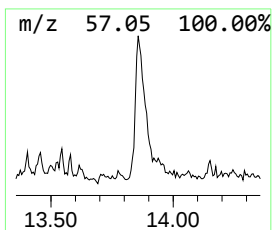
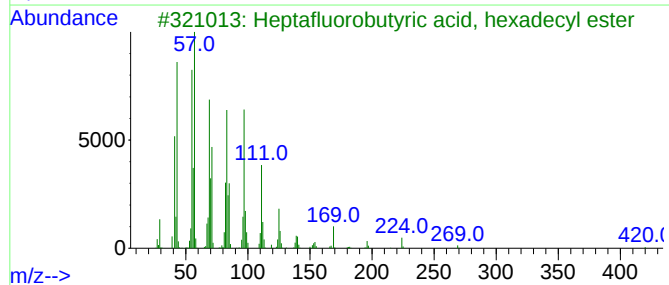
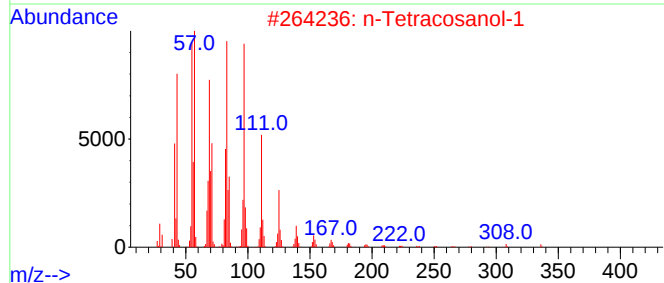
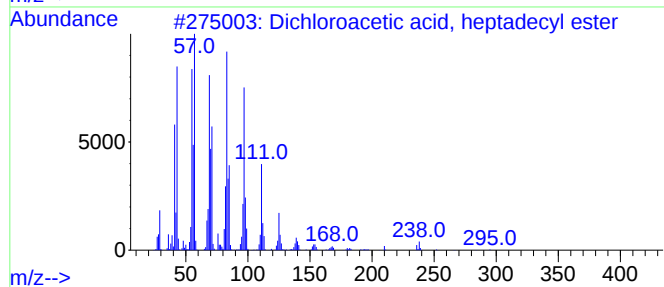
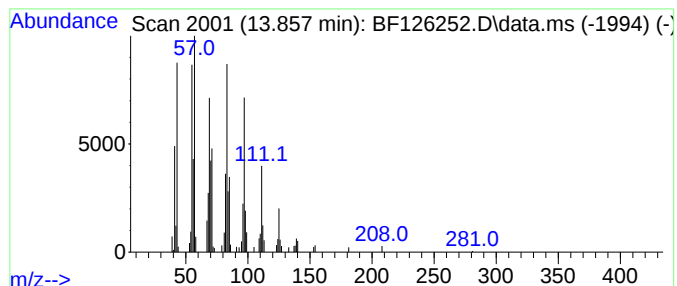
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Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	5.24 ng	412445	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.028	24.2	ng	1593550	1	6.816	1319350	20.0
2-Pentanone, 4-...	5.828	2.5	ng	166442	1	6.816	1319350	20.0
Dichloroacetic ...	13.857	5.2	ng	412445	5	13.974	1574580	20.0