

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112420\
 Data File : BP004085.D
 Acq On : 24 Nov 2020 20:25
 Operator : CG/JU
 Sample : L4588-01 5X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 HD-02-112320

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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-BP110320.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.923	3	6	22	rVB	1346555	1795882	100.00%	12.229%
2	3.076	26	32	41	rVV	55439	116388	6.48%	0.793%
3	3.170	44	48	55	rVB	47484	67873	3.78%	0.462%
4	5.805	488	496	507	rBV	274136	430797	23.99%	2.933%
5	7.452	769	776	789	rBV	256912	447470	24.92%	3.047%
6	8.264	908	914	924	rBV	480810	794738	44.25%	5.412%
7	9.428	1098	1112	1120	rBV	162969	289258	16.11%	1.970%
8	11.099	1386	1396	1406	rBV	627655	1097948	61.14%	7.476%
9	12.493	1625	1633	1640	rBV	19655	37650	2.10%	0.256%
10	13.428	1788	1792	1799	rVB4	12410	22353	1.24%	0.152%
11	13.510	1799	1806	1818	rBV	386810	586453	32.66%	3.993%
12	13.704	1834	1839	1846	rBV2	30425	55525	3.09%	0.378%
13	14.316	1938	1943	1948	rBV	18634	39380	2.19%	0.268%
14	14.763	2016	2019	2026	rVB	31255	39540	2.20%	0.269%
15	14.893	2030	2041	2053	rBV	903958	1429080	79.58%	9.731%
16	15.704	2176	2179	2185	rVB	36352	48048	2.68%	0.327%
17	16.375	2287	2293	2306	rBV	252060	393453	21.91%	2.679%
18	16.563	2321	2325	2328	rBV	36721	52281	2.91%	0.356%
19	16.593	2328	2330	2334	rVB	31346	37895	2.11%	0.258%
20	17.351	2455	2459	2464	rBV	36157	45992	2.56%	0.313%
21	17.410	2465	2469	2473	rVV2	29659	39093	2.18%	0.266%
22	17.622	2499	2505	2511	rBV	1133632	1586436	88.34%	10.803%
23	18.075	2579	2582	2585	rBV	39215	47882	2.67%	0.326%
24	18.239	2606	2610	2615	rVB	123933	150740	8.39%	1.026%
25	18.734	2691	2694	2699	rVB	30062	35217	1.96%	0.240%
26	19.316	2789	2793	2795	rBV	178082	219285	12.21%	1.493%
27	19.345	2795	2798	2802	rVB	712629	779580	43.41%	5.308%
28	19.475	2816	2820	2825	rBV	78527	106309	5.92%	0.724%
29	19.598	2838	2841	2845	rBV	45903	53873	3.00%	0.367%
30	19.945	2897	2900	2908	rVB	63801	103206	5.75%	0.703%
31	20.116	2925	2929	2934	rVB	647844	759795	42.31%	5.174%
32	21.657	3186	3191	3196	rBV	1185925	1542107	85.87%	10.501%
33	24.133	3607	3612	3620	rVB2	724641	1434194	79.86%	9.766%

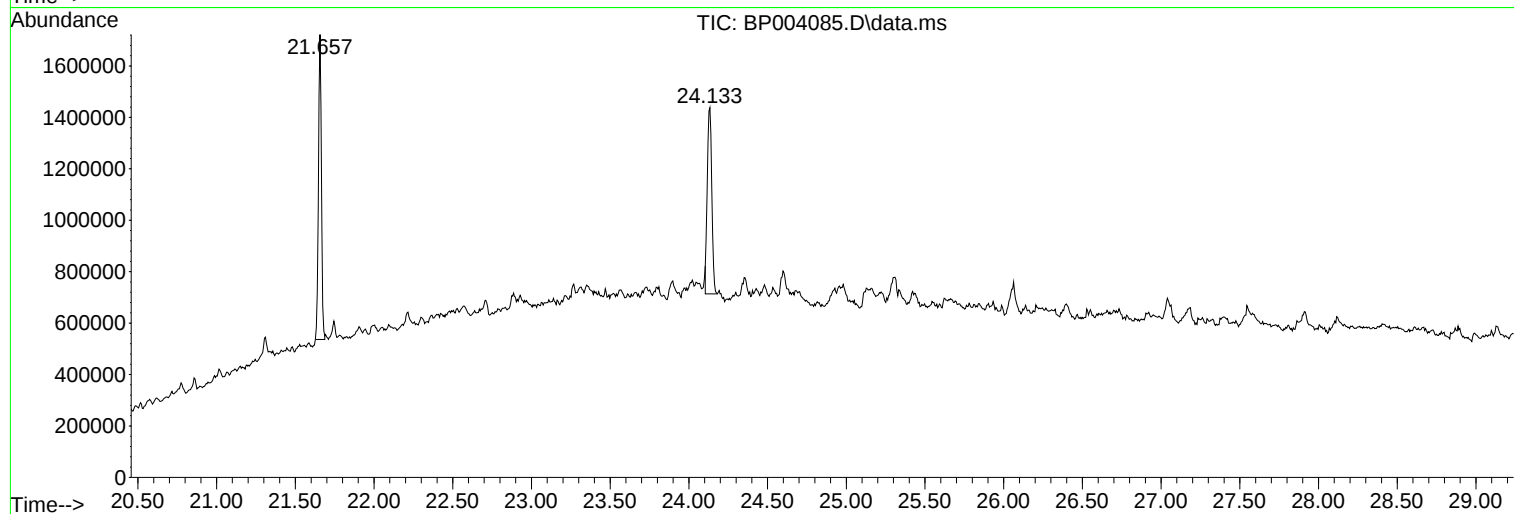
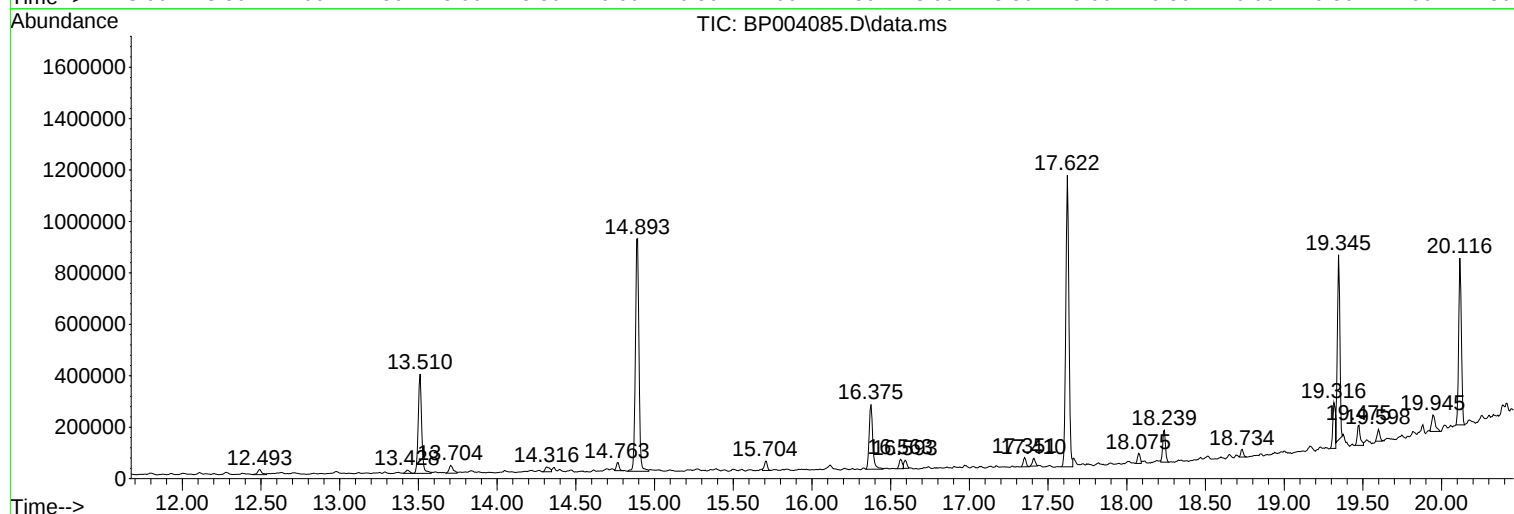
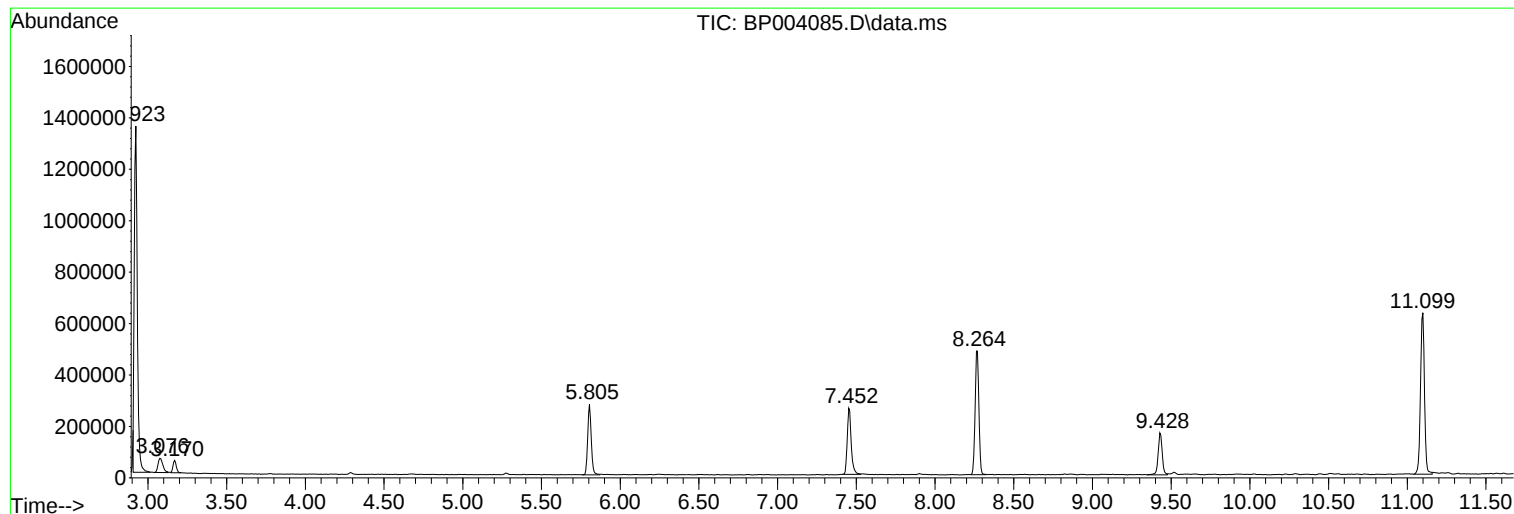
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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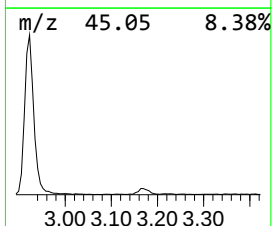
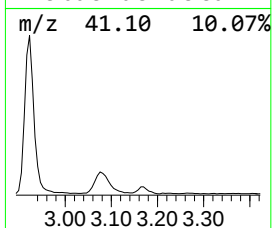
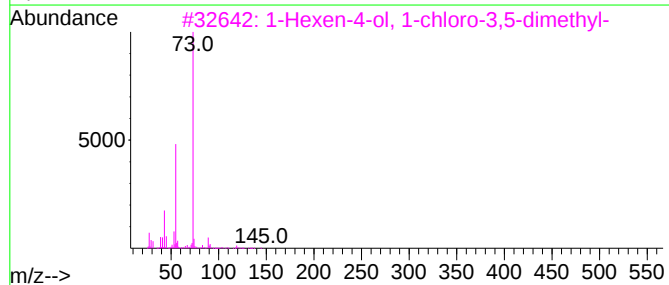
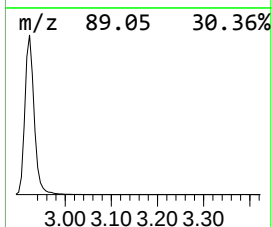
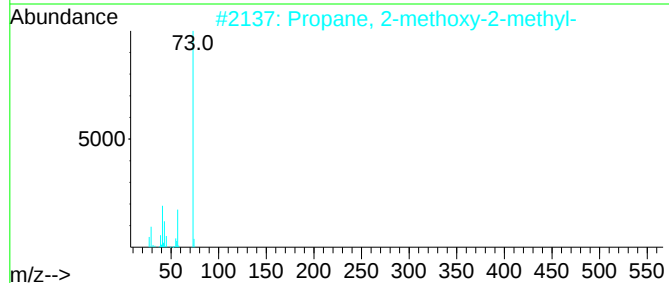
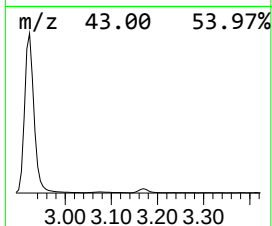
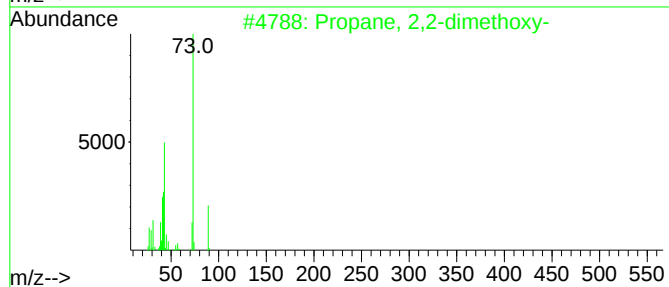
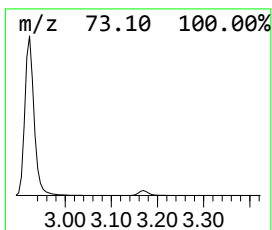
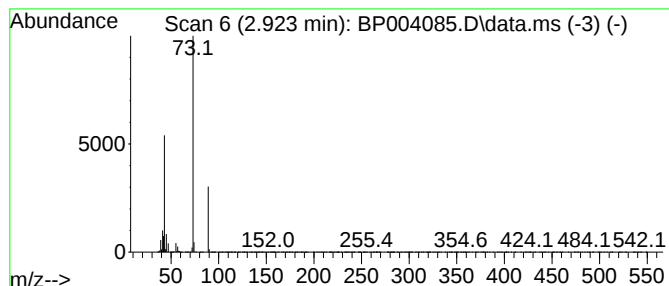
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.923 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.923	45.19 ng	1795880	1,4-Dichlorobenzene-d4	8.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3			1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	7



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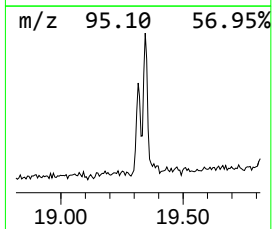
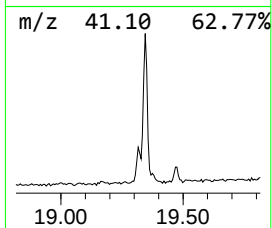
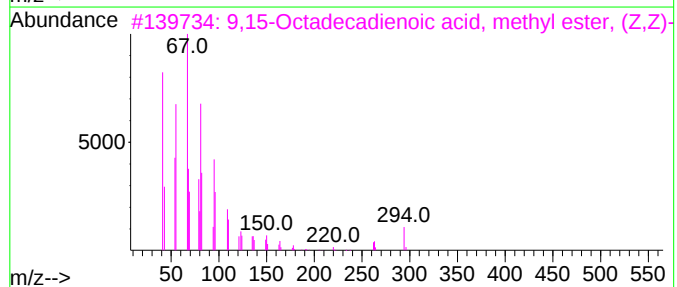
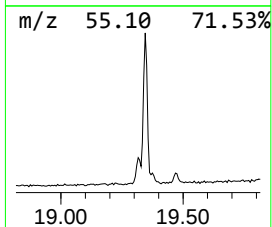
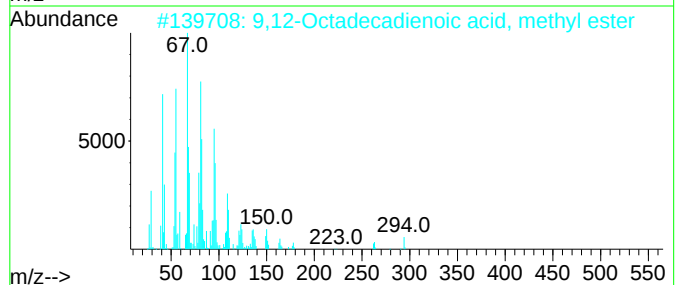
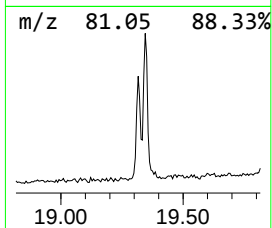
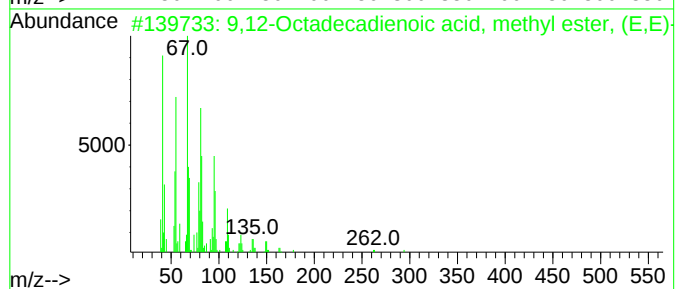
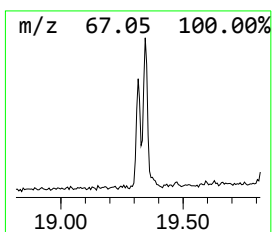
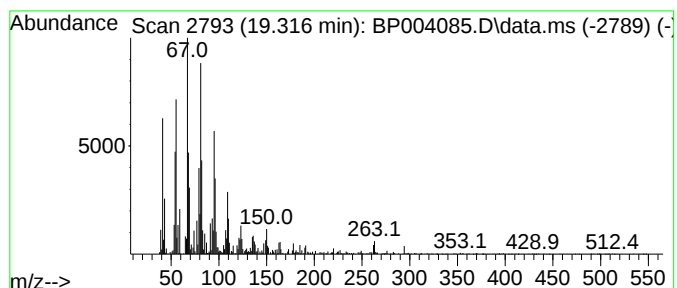
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.316	2.76 ng	219285	Phenanthrene-d10		17.622	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...		294	C19H34O2	017309-05-6	98
4	9,12-Octadecadienoic acid (Z,Z)-...		294	C19H34O2	000112-63-0	95
5	8,11-Octadecadienoic acid, methy...		294	C19H34O2	056599-58-7	94



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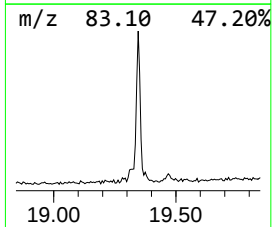
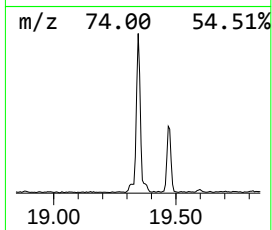
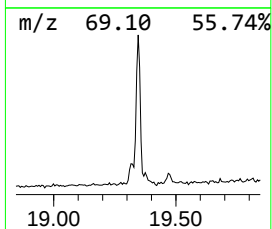
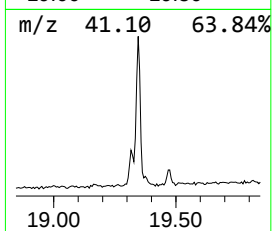
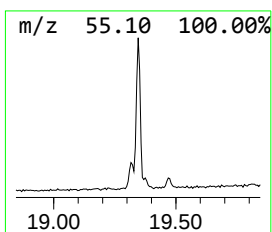
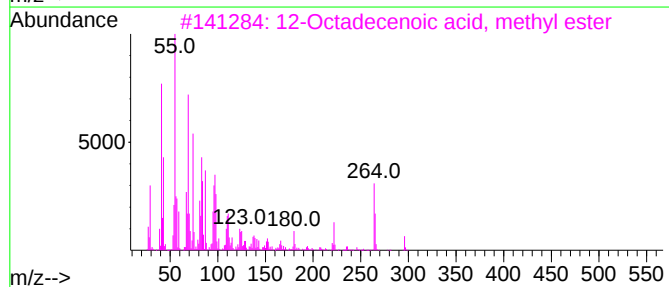
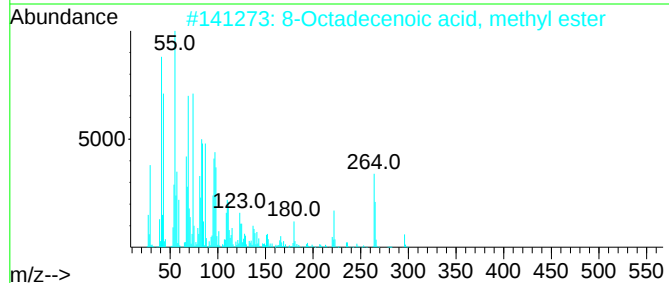
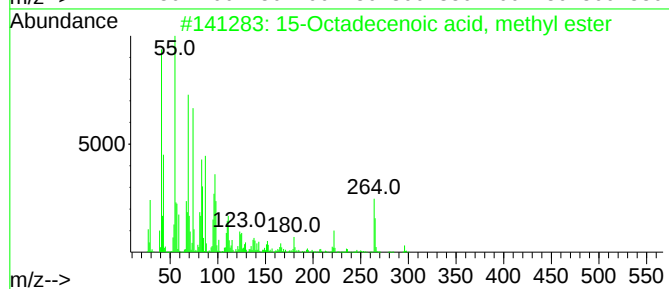
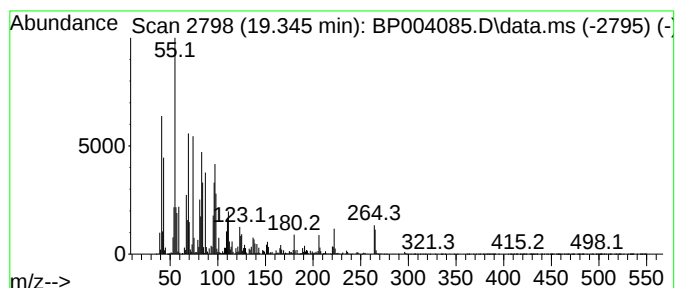
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 15-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.345	9.83 ng	779580	Phenanthrene-d10	17.622	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
2	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
3	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
4	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	98
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	97



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.923	2.923	45.2	ng	1795880	1	8.269	794738	20.0
9,12-Octadecadi...	19.316	2.8	ng	219285	4	17.622	1586440	20.0
15-Octadecenoic...	19.345	9.8	ng	779580	4	17.622	1586440	20.0